Green Energy and Technology

Ibrahim Dincer
Janette Hogerwaard
Calin Zamfirescu

Clean Rail Transportation Options

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Ibrahim Dincer • Janette Hogerwaard
Calin Zamfirescu

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Ibrahim Dincer
Janette Hogerwaard
Calin Zamfirescu
Department of Automotive, Manufacturing
and Mechanical Engineering
Faculty of Engineering and Applied Science
University of Ontario Institute of Technology
Oshawa, Canada

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Preface

The extensive use of fossil fuel in railway transportation is a high concern in North America and other world regions where diesel and/or diesel-electric locomotives represent the majority of prime movers. Besides rail transport, a major emission source of greenhouse gases is road transportation, which relates practically to gasoline and diesel fuels. As an example, in Canada, the transportation sector is the largest contributor to greenhouse gas emissions with over 25 % of the total emissions. Reduction of these emissions for the benefit of better and clean air and environment requires, among others, a strong encouragement of public transit, especially of rail transport. This obviously implies development and implementation of a clean rail transportation infrastructure.

This book discusses the current status and historical overview of rail transport and rail transport systems and applications and the development of alternative system and fuel options for a clean rail sector, which relates to sustainable energy sources and fuels, and thus produces substantially less pollution than the conventional railway which is in place today. Various cleaner fuels were considered in the past, among which one notes natural gas (in compressed or liquefied forms), methanol and biodiesel or other diesel fuel blends, hydrogen, and more recently ammonia. Purely electric rail transport remains a major option, which although being expensive, may be the preferred solution for some jurisdictions relating on clean power generation (e.g., hydro, wind, nuclear).

This book comprises nine chapters. After the introductory chapter, the rail transportation outlook is provided in Chap. 2, with emphasis on rail transport, rail status, and railway environmental impact. The conventional locomotive prime movers are presented in Chap. 3, with a historical perspective aimed at presenting the evolution of technical concepts and economic drivers from the beginning of the railways (in the 1700s) until the present. Chapter 4 presents the existing clean fuels options for railways, analyzing their main properties and mentioning the fuel fabrication pathways in a sustainable manner. The worldwide initiatives on the Clean Rail development are summarized in Chap. 5. Some relevant emerging locomotive systems for clear rail applications are reviewed in Chap. 6, with a focus on hydrogen, natural gas, and ammonia locomotives as the main three pillars. Chapter 7 presents the methods of locomotive assessment based on multiple criteria including thermodynamic analyses and assessment with energy and energy methods, as well as the economic, environmental, and sustainability assessment. The book comprises a number of case studies for actual systems with focus on a multi-criteria comparative assessment with a baseline case of diesel-electric locomotive as presented in Chap. 8. The main concluding remarks are summarized and some recommendations are made in Chap. 9. The book comprises a comprehensive list of references and technical appendices with relevant data for analyses.

Before closing, the authors sincerely acknowledge the financial support provided by Transport Canada, which is leading the Government of Canada's efforts to reduce rail sector emissions by supporting research of new and emerging technologies, under the Clean Rail Academic Grant Program.

Oshawa, Ontario

Ibrahim Dincer
Janette Hogerwaard
Calin Zamfirescu

Contents

Nomenclature

Symbols

a_{st}	Molar air-fuel ratio
AF	Mass-based air-fuel ratio
C_o	Reference cost, $
D_p	Depletion factor
$\dot{E}$	Energy rate, kW
EF	Emission factor
ex	Specific exergy, kJ/kg
$\dot{E}x$	Exergy rate, kW
$ExDR$	Exergy destruction
f_c	Conversion factor
GF	Greenization factor
h	Specific enthalpy, kJ/kg
$\dot{H}$	Enthalpy rate, kW
M	Molar mass, kg/kmol
$\dot{m}$	Mass flow rate, kg/s
P	Pressure, kPa
pr	Pressure ratio
$\dot{Q}$	Heat rate, kW
s	Specific entropy, kJ/kg K
SI	Sustainability index
T	Temperature, °C or K
v	Specific volume, m^3/kg
V	Volume, m^3 or L
$\dot{V}$	Volume flow rate, m^3/s
$\dot{W}$	Work rate, kW
x	Vapor quality
x_d	Dissociation fraction

Greek Letters

Δ	Difference
η	Energy efficiency
ρ	Density, kg/m^3
φ	Equivalence ratio
ψ	Exergy efficiency

Subscripts

1,2,…,i	State points
a	Air
ac	Aftercooler
b	Brake
c	Cooling
C	Compressor
cc	Combustion chamber
d	Destruction
e	Exit
ec	Engine cooling
el	Electric
eq	Equivalent
eqp	Equipment
exh	Exhaust
i	Inlet
P	Pump
PC	Purchase cost
rec	Recovery
s	Isentropic
sh	Shaft
SM	Starter motor
st	Stoichiometric
T	Turbine
TM	Traction motor
TP	Traction power
u	Utilization
wjc	Water jacket cooling

Superscripts

ch	Chemical
ph	Physical

Acronyms

BATT	Battery
BHP	Brake horsepower
BSFEi	Brake specific fuel emissions of species i
$C_{12}H_{23}$	Diesel fuel
CAC	Criteria air contaminant
CH_4	Methane
CI	Compression ignition
CN	Canadian National
CNG	Compressed natural gas
CO	Carbon monoxide
CO_2	Carbon dioxide
COP	Coefficient of performance
DSU	Decomposition and separation unit
EMD	Electromotive diesel
EPA	Environmental Protection Agency
EXP	Expansion valve
FFE	Feed-plus-fuel energy
GOV	Engine governor
GEN	Generator
GHG	Greenhouse gas
GTA	Greater Toronto Area
GWP	Global warming potential
H_2	Hydrogen
HC	Hydrocarbon
HCCI	Homogeneous charge compression ignition
HEP	Head end power
HHV	Higher heating value
HPDI	High pressure direct injection
HRR	Heat recovery rate
HX-ac	Aftercooler

HX	Heat exchanger
ICE	Internal combustion engine
IPCC	Intergovernmental Panel on Climate Change
LEM	Locomotive Emissions Monitoring
LHV	Lower heating value
LNG	Liquefied natural gas
LPG	Liquefied petroleum gas
LPI	Low pressure injection
MOU	Memorandum of understanding
MSDS	Material safety data sheet
NG	Natural gas
N_2	Nitrogen
N_2O	Nitrous oxide
NH_3	Ammonia
NO_x	Nitrous oxide
O_2	Oxygen
ORC	Organic Rankine cycle
PAX	Passenger
PM	Particulate matter
RAC	Railway Association of Canada
RES	Reservoir/storage tank
RTK	Revenue tonne-kilometre
RC	Rankine cycle
S	Sulfur
SCR	Selective catalytic reducer
SM	Starter motor
SO_x	Sulfur oxide(s)
TC	Turbocharger
THP	Traction horsepower
TM	Traction motor
ULSD	Ultra low sulfur diesel
US	United States
WHO	World Health Organization

Chapter 1
Introduction

1.1 Growth of Population and the Energy Outlook

Since historical times world civilization has strived to develop being in a continuous quest for vital resources. Crises and declines of societies have alternated with periods of fruitful development. The world populations have reshaped continuously conquering more territories and developing knowledge and technologies. At any times along the history, humans have not only strived to accommodate with the environment but also to reshape the environment to better suit their needs. This is how human settlements have occurred and further developed over time in towns, cities, countries, and geopolitical regions. The humankind population has continued to increase and will do so according to the projections. Figure 1.1 shows the historical data and prediction of world population (BC—Before Christ, AD—Anno Domini). The population grows in about an exponential rate as the technology develops. It is projected that by 2050, the world population will reach about 10 billions of inhabitants [1].

The increase in population leads definitely to an increase in commodity demand. The most comprehensive way to analyze the commodity demand of the society is through energy. This is due to the fact that energy supply is at the base of the majority of humankind activities. Energy demand increase as population increases, as shown in Fig. 1.2. The energy demand depends on the population density and the economic development of the world region. The main world economic regions and their predicted energy demand by 2040 are shown in Fig. 1.3. This energy demand prediction can be appreciated for each of the major sectors of activity as shown in Fig. 1.4.

The style of living becomes an important element to consider, when the energy consumption is analyzed. The lifestyle in some world regions, having better economic development, leads to higher energy consumption per capita. The chart shown in Fig. 1.5 illustrates that the European countries and North America have the highest energy consumption per capita in the residential sector. This is predicted

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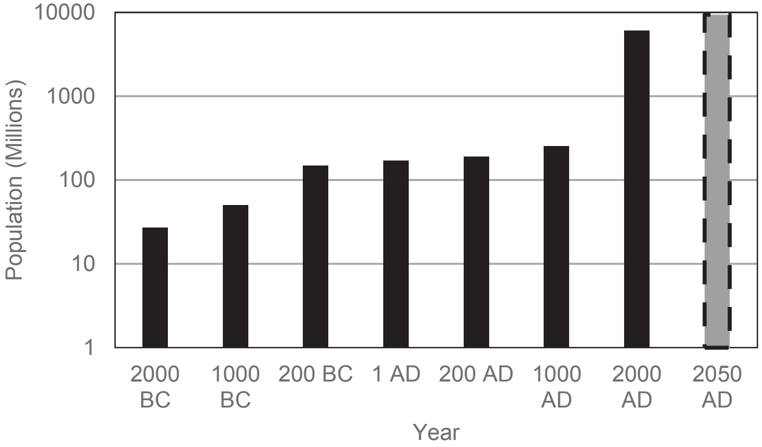


Fig. 1.1 World population statistics and projection *(dashed line/grey shaded)*. (Data from [1])

to decrease in North America; however, the predictions show that the residential energy per capita will increase in the non-Organisation for Economic Co-operation and Development (OECD) European countries. Overall, the world energy consumption per capita in the residential sector will increase, showing that the humans tend to enhance their lifestyle toward higher energy consumption.

Liquid fuels are the main source for transportation vehicles. Other uses of liquid fuels are in industrial sector and relatively less uses in residential and commercial sectors. The predicted trend of liquid fuel consumptions is shown in Fig. 1.6 for OECD and non-OECD countries. It is an apparent observation that the fuel consumptions tend to increase worldwide. For example, at present, the OECD countries consume more liquid fuel than non-OECD countries, but this situation is likely to

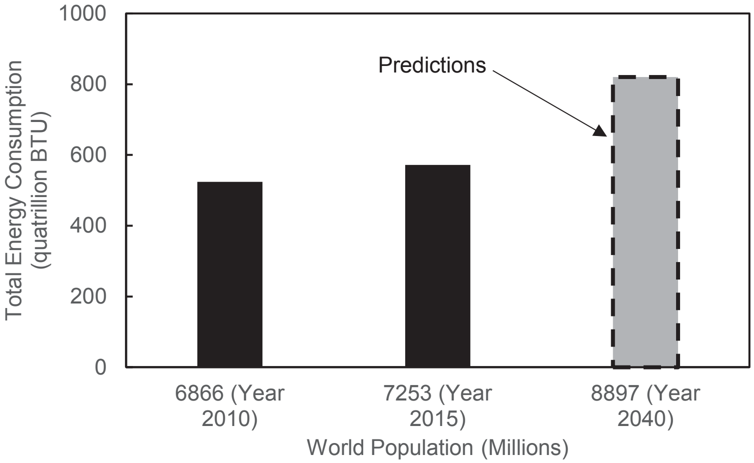


Fig. 1.2 Correlation between world population and energy consumption. (Data from [2])

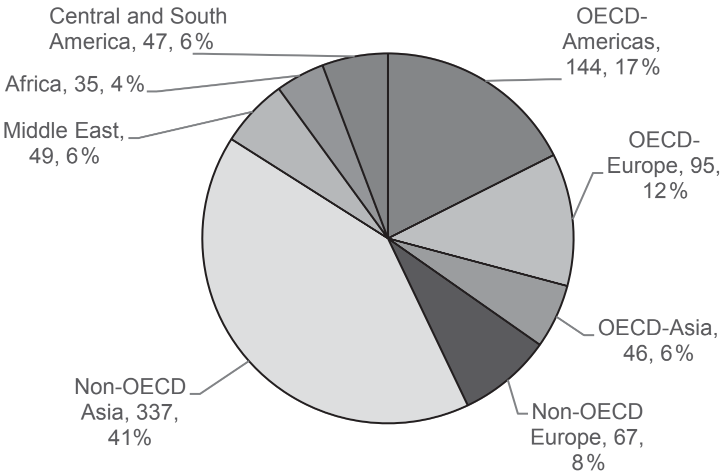


Fig. 1.3 Predicted energy demand by world region for 2040. (Data from [2]; energy in EJ)

be reversed in the future. The predicted trend of liquid fuel consumption per sector of activity is shown in Fig. 1.7. It clearly appears that transportation is the highest consumer of liquid fuels. The trend is that the liquid fuel demand in transportation sector will increase. The predicted increase is 30% with respect to year 2010 as baseline for transportation sector.

An increase in fossil fuel combustion leads to an increase in greenhouse gas (GHG; e.g., CO_2) emissions in the atmosphere, this being an alarming situation with respect to environmental impact and global warming. Figure 1.8 shows the carbon dioxide emission records and predictions caused by combustion of the three major fossil fuels: liquid petrochemical fuels, natural gas, and coal. All these types of

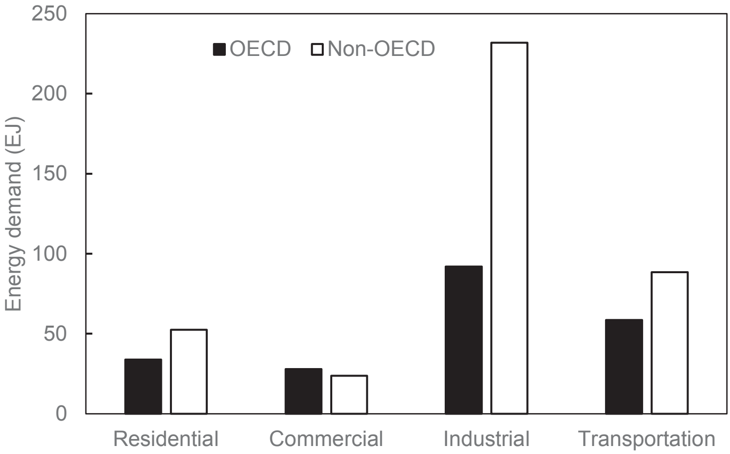


Fig. 1.4 Predicted energy demand of main activity sectors in 2040. (Data from [2])

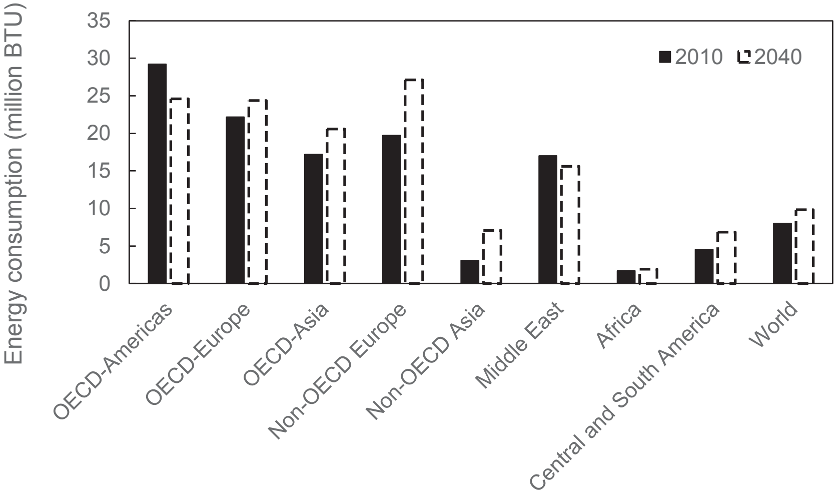


Fig. 1.5 Recorded (2010) and predicted (2040) residential energy consumption per capita in the main economic regions of the world. (Data from [2])

emissions tend to increase as predicted, with the fact that coal is treated as responsible for the majority of this type of atmospheric pollution.

Regarding the distribution of carbon dioxide emissions among OECD and non-OECD countries, this can be observed in the bar chart shown in Fig. 1.9. Although the OECD countries were responsible, in the past, for the majority of emissions, this situation is nowadays reversed. The predicted trend is that by 2040, the GHG emissions by non-OECD countries will be more than double with respect to OECD countries.

In brief, the situation depicted by the above-presented tendencies of increase in world population, standards of life, and energy consumption is quite alarming. The

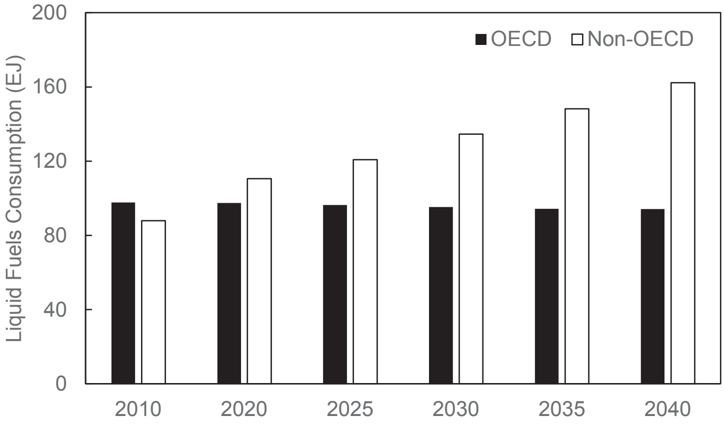


Fig. 1.6 Predicted trend of liquid fuel consumption. (Data from [2])

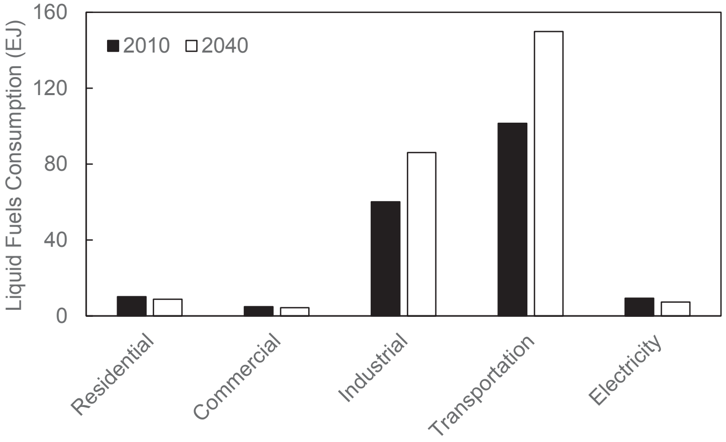


Fig. 1.7 Predicted trend of liquid fuel consumption per sector of activity. (Data from [2])

fossil fuels tend to deplete; in addition, these fuels are non-uniformly distributed in the world. As known, most petroleum resources are in Middle East; also, the approximated distribution of coal resources is as shown in Fig. 1.10. Apparently all coal and other mineral reserves will deplete since the consumption rate tends to increase and the resources are finite. The proven reserves of coal, petroleum, natural gas, and nuclear minerals are shown in Fig. 1.11. As a matter of fact, coal reserves are not only the most abundant but also their use leads to the most of carbon dioxide emissions into the atmosphere.

The ratio between fuel reserve and its current demand rate represent a time interval which signifies the resource availability. The mineral resource availability in

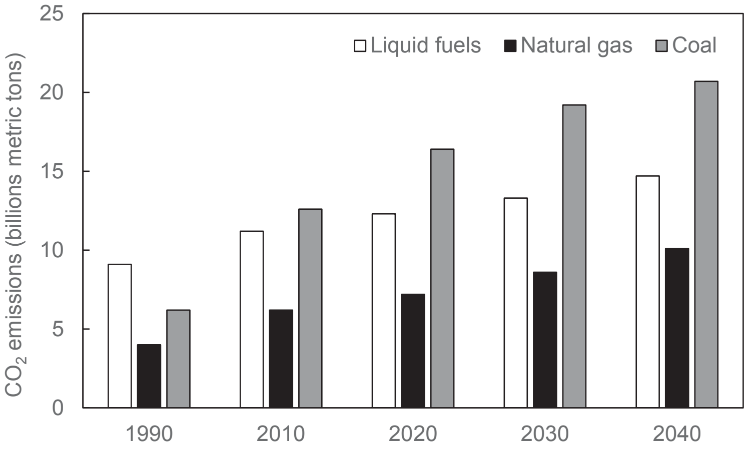


Fig. 1.8 Records and predictions of carbon dioxide emissions due to liquid fuel, natural gas, and coal combustion. (Data from [2])

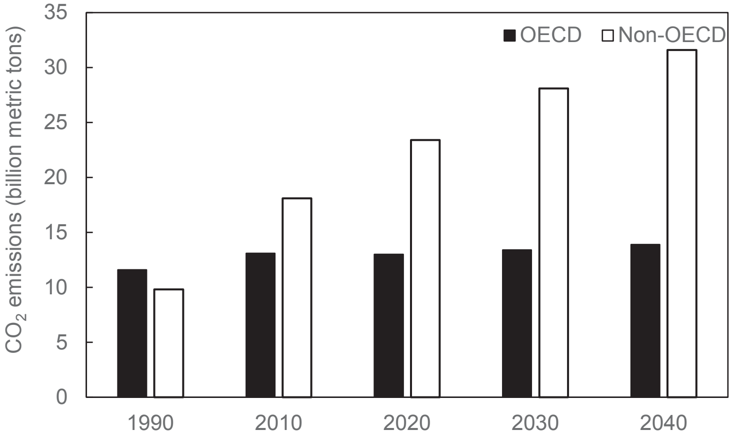


Fig. 1.9 Records and predictions of carbon dioxide emissions due to fossil fuel combustion for OECD and non-OECD. (Data from [2])

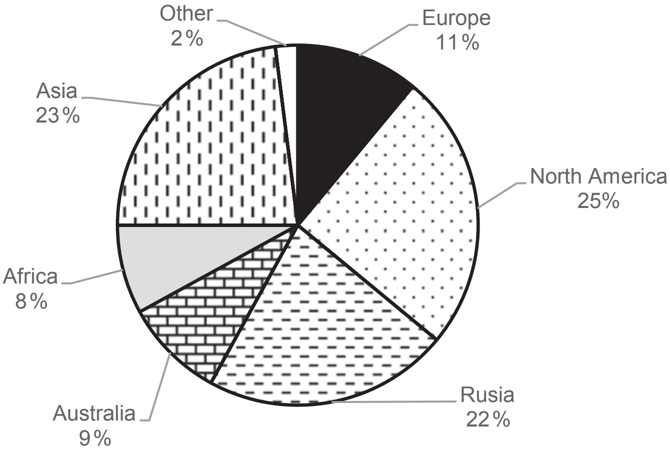


Fig. 1.10 Worldwide distribution of coal reserves. (Data from [3])

Table 1.1 Predicted availability of mineral resource. (Source: [3])

Resource	Coal	Petroleum	Natural gas	Uranium
Availability (years)	122	42	60	50

years is given in Table 1.1. With the current demand and proven resource, petroleum fuels (mainly liquids) will last the least, whereas the coal will last the longest (for 122 years).

Some prediction equations are available in the literature for energy consumption from the main types of fossil fuels. These are given here from [4] where an artificial

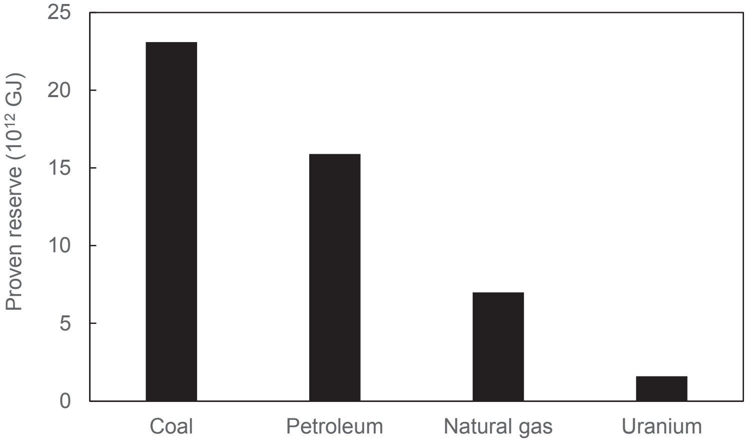


Fig. 1.11 Proven reserves of mineral fuels. (Data from [3])

neural network modeling technique can be used to correlate the data. Based on the curve fitting to correlate the data, some useful correlations are developed to make future projections based on the past actual data. In this regard, coal energy demand is predicted according to the following correlation:

$$E_{\text{coal}}\,(\text{EJ}) = 125.6667\left[1+\exp\left[-\left(\frac{Y-1968.0551}{24.2314}\right)\right]\right]^{-1} \text{ and } (R^2 = 0.99998) \tag{1.1}$$

where E_{coal} denotes world coal consumption in EJ and Y is the year, and R is the mean square error. The world oil consumption curve correlation with the correlation coefficient is utilized as follows:

$$E_{\text{oil}}\,(\text{EJ}) = 184.5575\left[1+\exp\left[-\left(\frac{Y-1987.7137}{10.2282}\right)\right]\right]^{-1} \quad \text{and} \quad (R^2 = 0.99947) \tag{1.2}$$

The correlation developed for the world natural gas consumption curve is given with the correlation coefficient as follows:

$$E_{\text{ng}}\,(\text{EJ}) = 186.5923\left[1+\exp\left[-\left(\frac{Y-1984.2525}{27.0821}\right)\right]\right]^{-1} \quad \text{and} \quad (R^2 = 0.99965) \tag{1.3}$$

The global demand for energy services is expected to increase by as much as an order of magnitude by 2050, while primary energy demands are expected to increase by 1.5–3 times. Trying to predict the evolution of world energy market, policymakers studied various long- and short-term scenarios. A relevant work in this respect has been pursued by the European Commission in [5] that gives the world energy technology outlook up to 2050. In the report, the geopolitical context, CO_2 emission profile, oil, gas, and coal production profiles, renewable energy technology development, population growth, predicted energy demand, and other aspects are accounted for to propose a number of scenarios for energy technology development up to 2050, shown in brief here in Fig. 1.12. It is recognized that the share of renewable and nuclear energy in total primary energy demand will increase, while the share of fossil fuels will decrease. The major renewable energy source used by 2050 will be biomass, followed by wind and solar, and then by hydro- and geothermal energies.

1.2 Environmental Impact of Anthropogenic Activities

The human activity has impact on the environment. Due to their activity, humans build and modify the landscape and the terrestrial environment. Building dams, roads, and cities and doing deforestation are examples of anthropogenic impact on the environment. The combustion of fossil fuel is essentially considered harmful to the environment, as they are known as hydrocarbon fuels, due to their carbon content. Over the past few decades, energy-related environmental concerns have expanded from primarily local or regional issues to the international and global nature of major energy-related environmental problems.

Particularly in developing or newly industrialized countries, where energy consumption growth rates are typically extremely high and where environmental management has not yet been fully incorporated into the infrastructure, environmental problems are becoming apparent or already exist. Nevertheless, at present, mainly

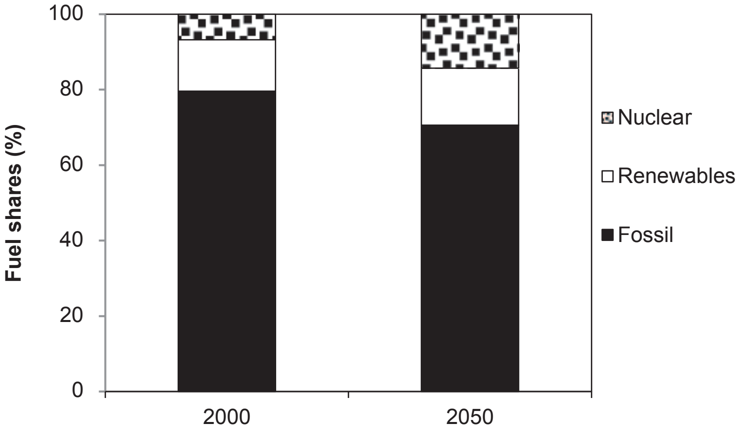


Fig. 1.12 Shares of fossil fuel, nuclear, and renewable energy resource demands in year 2000 and predictions for year 2050. (Data from [5])

industrialized countries are responsible for air pollution, ozone depletion, and the carbon emissions. There may be pollutant emissions, accidents, hazards, ecosystem degradation through air and water pollution, animal poisoning, GHG emission, carbon monoxide leakages, stratospheric ozone depletion, emission of SO_2, NO_x, volatile organic compounds (VOCs), particulate matter (PM), other aerosols, etc.

The effluents expelled in the atmosphere by power generation systems can be categorized into two kinds: GHGs and aerosols. GHGs are those chemicals which are released in the terrestrial atmosphere and produce *greenhouse effect*. When released from natural and anthropogenic activities, GHGs travel through the atmosphere and reach its upper layer, the *troposphere*. At the troposphere level, GHGs absorb an important part of the infrared radiation emitted by the earth surface. As a consequence, the earth surface temperature tends to increase, and this process is called the *greenhouse effect*.

On the other hand, aerosols such as VOCs, soot, and PM, etc. are released continuously in the atmosphere and concentrate at its upper layers. Aerosols contribute to the earth's *albedo*. Due to their presence in the atmosphere, aerosols reflect and scatter back in the extraterrestrial space a part of the incident solar radiation. As a matter of consequence, the earth temperature tends to decrease. This process is termed as *albedo effect*. The balance between greenhouse and albedo effects establishes the earth temperature and regulates the earth climate. This mechanism of climate control is a natural process. However, it is noted that since the industrial revolution, the anthropogenic impact on climate became obvious due to accentuated emission of GHGs emitted massively by many activity sectors (energy, transportation, industry) which induce a tendency of *global warming*. Global warming leads to changes in natural systems. There is an increased melting effect of permafrost ice, and consequently, there is a continuous tendency of sea level increase. Moreover, there are observed changes in global precipitations (with more dry areas and more regions flooding), and there have been recorded a number of extreme events (tsunami, extreme winds, etc.).

Another major environmental impact induced by energy systems is due to acid precipitations. Gaseous effluents expelled in the atmosphere by power generation systems can eventually form acids and with precipitations these return back on earth contributing in acidification of soil and seas. This effect negatively affects all life systems. Other impacts are also possible as will be detailed subsequently. The main types of pollutant emissions due to energy systems are listed in Table 1.2, and their influence is explained.

One of the most important environmental impact indicators is the global warming potential (GWP) measured in kilogram of CO_2 equivalent of GHGs emitted. The principal GHGs emitted in the atmosphere (except the water vapor) as listed in Table 1.2 are carbon dioxide, methane, and nitrogen dioxide. These gases are part of natural cycles of carbon and nitrogen and part of anthropogenic emissions; therefore, they were present in the atmosphere prior to the industrial era, for which the year 1750 is considered the reference. As seen in Fig. 1.13, the concentration of these gases in year 1750 is higher than zero. It is certain that atmospheric CO_2 levels will continue to increase significantly. The degree to which this occurs depends

Table 1.2 Atmospheric pollutants released by power generation systems

Pollutant	Description
GHG	Greenhouse gases: These are gases that produce greenhouse effect. The main GHGs are CO_2, CH_4, and N_2O. Greenhouse effect is the main cause of global warming
CO	Carbon monoxide: It arises mostly from the incomplete combustion of fuels and poses risk for health and life of animals and humans are at high risk upon inhalation. Intense emission of CO in open spaces may affect birds, whereas emissions in close spaces (residences, garages) may induce death of exposed persons
SO_2	Sulfur dioxide: It is a corrosive gas which is hazardous to human health and harmful to the natural environment. It results from combustion of coal and fuel oil, smelting of nonferrous metal ores, oil refining, electricity generation, and pulp and paper manufacturing. It causes respiratory difficulties, damages green plants, and is a precursor of acid precipitation
NOx	Nitrogen oxides (NO and NO_2): It is produced by combustion of fuels at high temperature in all combustion facilities from large scale to small scale (including motor engines, furnaces, etc.). It can lead to respiratory problems in humans and animals. It can form acids in high-altitude atmosphere
VOCs	Volatile organic compounds: These are volatile organic particles resulting from hydrocarbon combustion in engines and these have harmful effects in the atmosphere and impede formation of stratospheric ozone
PM	Particulate matter: Particles in the air (fly ash, sea salt, dust, metals, liquid droplets, soot) come from a variety of natural and man-made sources. Particulates are emitted by factories, power plants, vehicles, etc., and are formed in the atmosphere by condensation or chemical transformation of emitted gases. PM leads to health and environmental effects including acid precipitation, damage to plant life and human structures, loss of visibility, toxic or mutagenic effects on people, and possibly non-accidental deaths
CFC, HCFC, HFC	Chlorofluorocarbons: These are mainly refrigerants or propellants. They can contribute to the destruction of the stratospheric ozone layer and to greenhouse effect

on the fixture levels of CO_2 production and the fraction of that production which remains in the atmosphere. Given plausible projections of CO_2 production and a reasonable estimate which states that half the emitted amount will remain in the atmosphere, it is generally believed that sometimes during the middle of twenty-first century, the concentration of CO_2 will reach 600 ppm in the atmosphere.

The *radiative forcing* is defined as the net change in radiation balance at the tropopause, produced by a specified cause. By convention, if the radiative forcing is positive then it induces an increase of planet temperature, and if it is negative then vice versa. The unit of measure of radiative forcing is the same as the unit of radiation energy rate per square meter of earth surface, where the earth surface, by convention, is the area of the sphere having the average radius of the planet. The usual symbol for the radiative force is ΔF, and typical values range from 0 to 2 W/m^2. It can be derived from what was explained above that change in the concentration of

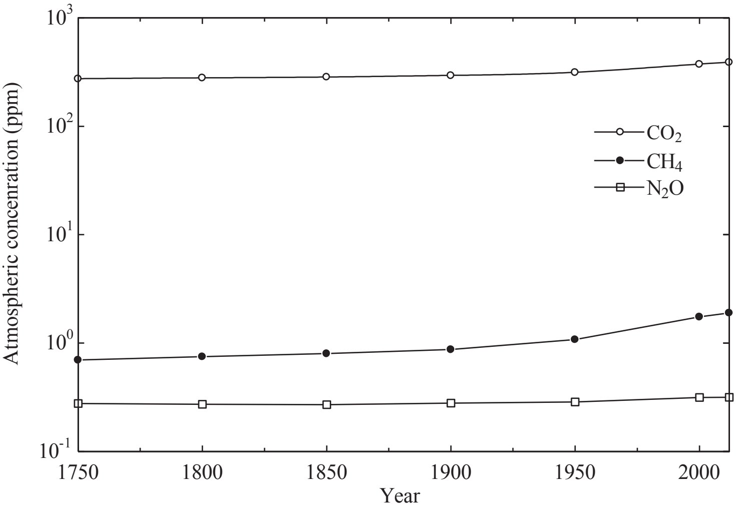


Fig. 1.13 Evolution of atmospheric concentration of main GHGs starting with industrial revolution. (Data from [6])

GHGs, aerosols, and atmospheric ozone induces radiative forcing. Depending on the concentration of the gas in the atmosphere, there are three regimes of producing radiative forcing: low, moderate, and high concentration.

Quantifying the effect on climate that a particular atmospheric gas has is a multivariable problem. On one side, the radiative forcing induced by the respective in an indication of the direction in which the presence of the respective gas can influence the climate. If, for example, the gas absorbs more in infrared spectrum, its greenhouse effect is accentuated; that is, it has associated a positive radiative forcing. However, another parameter is also important, that is, the atmospheric lifetime. It is important how long the gas is active in the atmosphere with respect to radiative balance control. The net forcing produced during an infinitesimal time interval is given by the product $\mathit{\Delta F}_{\mathrm{CO_2}}(\mathrm{t})\cdot f_{\mathrm{CO_2}}(t)$, where we use the notation $f_{\mathrm{CO_2}}(t)$ to emphasize that the fraction of gas mass existent in the atmosphere is a function of time. One can integrate the former quantity over a time horizon *TH* and obtain the total forcing produced by the respective amount of $\mathrm{CO_2}$. If another kind of GHG except carbon dioxide is considered, its integrated forcing over the time horizon can be normalized with the integrated forcing of $\mathrm{CO_2}$. From this reasoning, it results in the following definition for the GWP of the GHG:

$$\mathrm{GWP}=\frac{\int_0^{\mathrm{TH}} \Delta F_{\mathrm{GHG}}(t) f_{\mathrm{GHG}}(t)dt}{\int_0^{\mathrm{TH}} \Delta F_{\mathrm{co_2}}(t) f_{\mathrm{co_2}}(t)dt} \tag{1.4}$$

Table 1.3 gives the GWP of main GHG for three time horizons. The evolution of atmospheric concentration of the main GHG based on historical records is presented in Fig. 1.13. This figure shows a continuous increase in emissions starting with industrial revolution and until present. Each of these gases has an effect to the radiative forcing proportional to its GWP.

Figure 1.14 presents the evolution of radiative forcing induced by the main three GHGs in the last 250 years. As it can be observed, radiative forcing and, thus, the climate are mostly influenced by carbon dioxide emissions, followed by methane and nitrous oxide emissions. It can be remarked that a correlation between radiative forcing increases due to GHGs emissions and the global temperature and sea level.

In Fig. 1.15, the recorded data of global temperature and sea level increase with respect to year 1870 are represented. According to [6], the satellite data show that in the last 35 years, the Arctic sea ice shrunk about 2.7 times. In the last 100 years, the global surface temperature increased about 0.74 K. The sea level increased about

Table 1.3 Principal GHGs and their GWP

Gas	Absorption spectrum, cm^{-1}	Atmospheric concentration	Atmospheric lifetime	GWP		
				20	100	500
CO_2	550–800	387 ppm	50–200 years	1	1	1
CH_4	950–1650	1750 ppb	12 years	72	25	7.6
N_2O	1200–1350	314 ppb	120 years	289	298	153

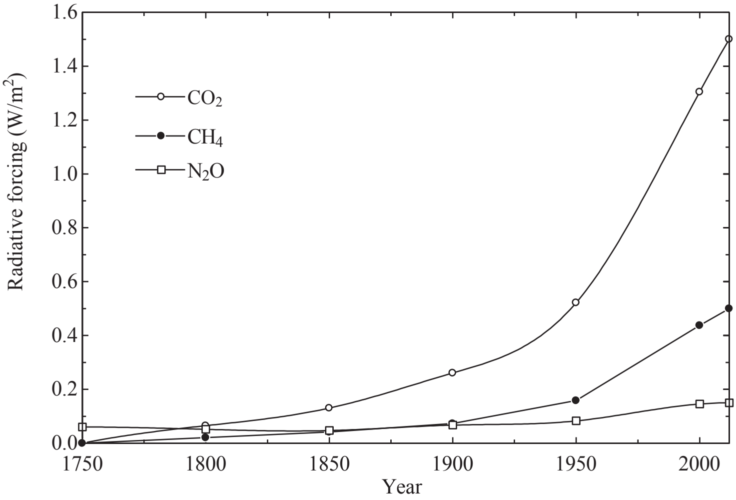


Fig. 1.14 Evolution of radiative forcing due to main GHGs starting with industrial revolution. (Data from [6])

0.2 m in the last 150 years. It is demonstrated that the recent records of global warming affect life systems on the earth and in oceans. From Figs. 1.14 and 1.15, it is visible that GHG emission from human activity increased sharply in the past 40 years.

Figure 1.16 shows the GHG emission by sectors of activity and by major GHG type. Human activities since the industrial revolution especially that related to fossil fuel combustion in industrial, commercial, residential settings and in transportation sector have dangerously impacted the global environment. It is clearly remarked from the figures that the transportation sector is responsible of a large share of GHG emissions in the atmosphere with 13 % share. As mentioned above, carbon dioxide emissions are the most important anthropogenic impact on global warming. Figure 1.16b reveals that among carbon dioxide sources, combustion of fossil fuels is the most important with 57 % of shares.

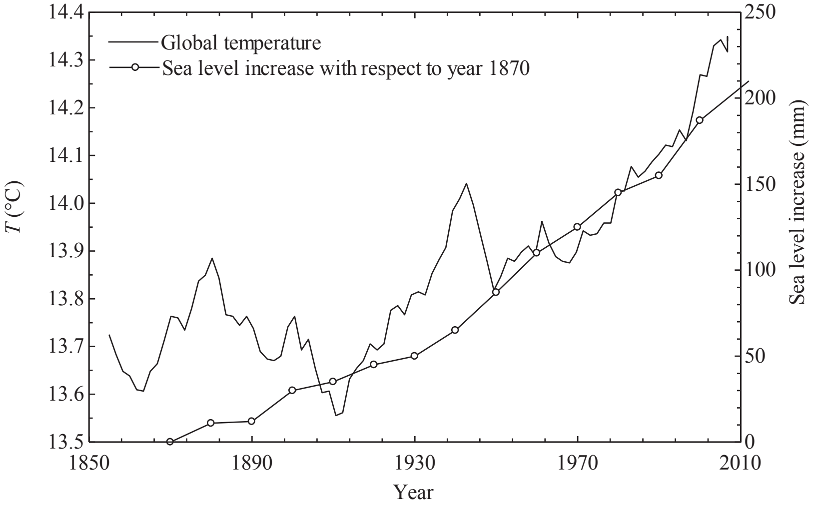


Fig. 1.15 Recorded temperature and sea level changes during the past 250 years. (Data from [6])

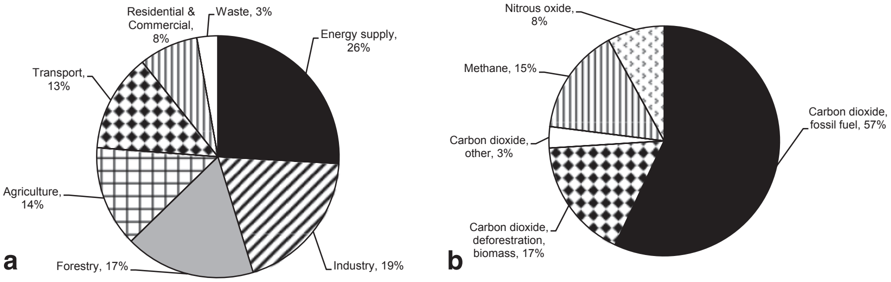


Fig. 1.16 Anthropogenic GHG emissions by sectors (**a**) and major gases (**b**). (Data from [6])

Regarding the effect which is the opposite of greenhouse effect—namely the albedo effect—this is caused by aerosols of which many are generated by energy supply sector. Black carbon, nitrates, soot, primary sulfates, organic carbon, VOCs, chlorides, ozone, and trace metals generate albedo. According to [6], a negative radiative forcing of at least —0.5 W/m^2 is due to the albedo effect, which is in unbalance with the radiative forcing of $\sim +1.5$ W/m^2 which is caused by the GHG emissions. This unbalance is expected to increase in the future as it is projected a more dramatic increase in GHG emissions. Prediction of GHG emission in the next 100 years is of major importance in shaping energy policy of today and promoting sustainable energy pathways. Depending on policy measure, it is possible to stop the increasing trend of GHG emissions at certain point in time. In such case, after reaching a maximum, the concentration of GHG in the atmosphere may decrease.

Emission of SO_2 and NO_x which characterizes the energy supply sector has a direct environmental impact due to acidification effect. These gases may participate in the complex set of chemical transformations in the atmosphere, resulting in acid precipitation. Road transport is also an important source of NO_x emissions. Most of the remaining NO_x emissions are due to fossil fuel combustion in stationary sources. Countries in which the energy-related activities mentioned here occur widely are likely to be significant contributors to acid precipitation. A major problem with acid rain is that its effects often occur in a different country than its source. There are a large variety of major evidences to show the damages of acid precipitation as follows:

- Acidification of lakes, streams, and groundwaters
- Toxicity to plants from excessive acid concentration
- Corrosion to exposed structures
- Resulting in damage to fish and aquatic life
- Damage to forests and agricultural crops
- Deterioration of buildings and fabrics
- Influence of sulfate aerosols on physical and optical properties of clouds

Economic priorities often cause land particularly suited for sustaining agriculture, housing, or natural ecosystems to be lost. In the energy sector, concern has focused on mining sites and hydroelectric reservoirs; the large land surfaces that might be needed for the large-scale exploitation of renewable energy forms, for example, solar power, wind power stations, or biomass production; the sites chosen for large, complex, industrial processes, for example, fuel refining or electric power generation; and the disposal of solid wastes including radioactive wastes.

Hazardous wastes pose special health and environment threats and are mainly generated by the chemical and metal industries. Nonhazardous wastes, for example, bottom ash from power plants and air-pollution control residues, pose disposal problems regarding space and appropriate containment. The commercial use of some solid wastes as building industry products and transportation surfaces is limited by the size of the market. Beside the environmental impact of energy systems on water and air quality, it can be observed at the level of ecosystems, food, coastal regions, industry, settlements, and health.

1.3 Sectoral Energy and Exergy Utilization

In a world with finite natural resources and large energy demands, it is important to understand mechanisms which degrade energy and resources and to develop systematic approaches for improving systems in terms of factors such as efficiency, cost, environmental impact, etc. The application of thermodynamic analysis at macroscale is simple to understand with the help of Fig. 1.17. As a first step, the thermodynamic system subjected to analysis must be delimited. For example, the thermodynamic system can be a sector of activity, such as industrial, commercial, transportation, agricultural, utility, etc.

The boundary of such system is fictive—it cannot be delimited physically, but rather the fluxes of energy/exergy in and out of the system under consideration can be inventoried. For the analysis to be done, a period of time must be specified, for example, 1 year and 1 season. The energy consumed by the system subjected to analysis can be determined based on the primary energy (or fuel sources) consumed over the specified period of time. The consumption of primary energy sources can be found from regional or national statistics.

At any macro-level (sector of activity, geopolitical region, country, etc.), statistics regarding the energy consumption by type (coal, natural gas, petroleum, etc.) and other useful information are issued regularly. For each fuel source, the higher or lower heating value can be used to convert the quantitative consumption (e.g., quantity by mass, mol, or volume) into energy or exergy terms. The useful energy or exergy is made available, depending on the case, in form of work, heat, electric power, chemicals (e.g., synthetic fuels, electric batteries) or other forms.

The difference between useful and consumed energy/exergy represents the energy loss or exergy destruction, respectively. Such energy/exergy balances can be written for any category of processes specific to the analyzed system. Based on

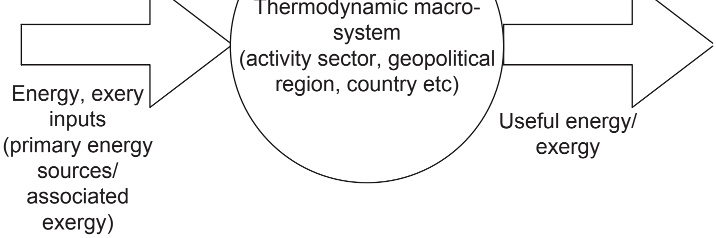


Fig. 1.17 Thermodynamic analysis at macroscale based on energy and exergy

inputs, outputs, and losses, energy and exergy efficiencies at macroscale can be defined, in analog manner to that commonly considered for any thermodynamic system.

The use of exergy in thermodynamic analysis at macroscale is of utmost importance. Consider, for example, petroleum oil and wood. Commonly, the first is perceived as fuel and the second as a construction material. Yet oil can be converted into a plastic material to be used for various purposes including in construction, and wood can be burned as fuel. At sectoral level, it is important to quantify the material fluxes and the associated exergy. As for any material, it can be determined a specific chemical exergy, one can realize that exergy is a measure that have the quality to unify the thermodynamic analysis. If one knows the energy carried by materials flows crossing the system boundary, the corresponding exergy can be determined through a quality factor. For example, if the flux of energy flows in form of heat, the quality factor is given by Carnot efficiency $1-\frac{T_0}{T_\mathrm{f}}$, where T_0 is the environment temperature and T_f is the temperature associated with the energy flux. If the flow of energy is in the form of electricity or work, the quality factor is 1.

The analysis made for each sector of activity which takes place in a specific geopolitical region can be compiled into a "sectoral energy/exergy flow diagram." An example of a diagram as such is presented in Fig. 1.18. There, a particular system is the utility, which generates electricity and delivers it to the grid. All other sectors are connected to the grid and also to the stream of primary energy/exergy fuel sources. In each sector, specific products and wastes are generated. Note that for each sector, there were specific processes that transform the energy input into useful products. For example, in residential sector, one can have space heating, water heating, cooking, electrical appliances, lighting, refrigeration and air conditioning, dish washing and ironing, television and computer, washing machine, vacuum cleaner, and others.

The waste from each sector includes pollutants, such as carbon dioxide emissions or other emissions, tars, residual, radioactive waste, and other kinds of wastes. Energy and exergy efficiency for all analyzed sector (complete geopolitical region) can be also derived by considering the overall energy and exergy output as a summation of those for each sector.

The industrial sector comprises many subsectors, of which the most important are iron-steel, other metallurgical subsectors, non-metal material subsector, chemical-petrochemical industry, fertilizer subsector, petrochemical feedstock subsector, and cement, sugar, and other industries. Figure 1.19 shows—as an example—the energy and exergy consumption from primary sources in Turkey.

The transportation sector comprises subsectors, namely roadway, railway, seaway, airway, and off-road transport for fuel and electricity consumption. The sector consumes, as main energy input, various types of fuels such as gasoline, compressed natural gas, fuel oil, kerosene, diesel oil, and hard coal. The use of coal in transportation sector is not direct; rather, coal is liquefied to obtain synthetic fuels in liquid phase. Electricity is also used to some extent for transportation, such as railways or metropolitan public transport. In the future perspective, hydrogen is be-

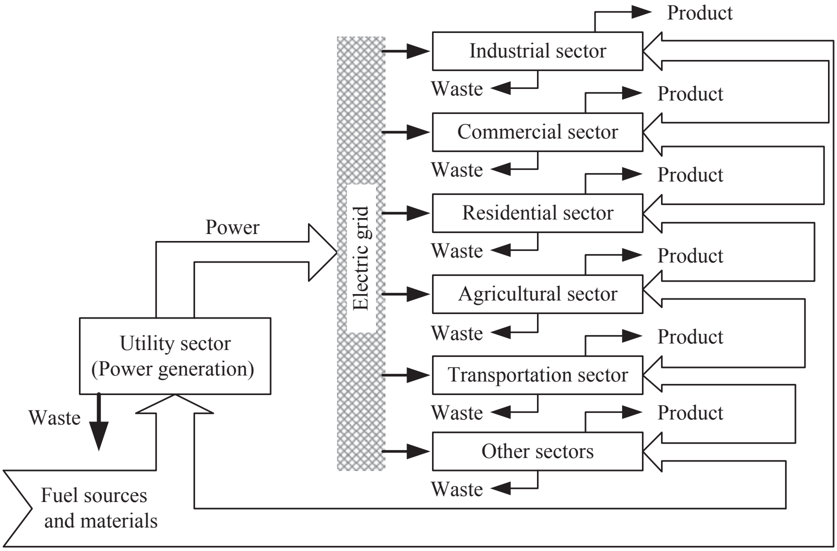
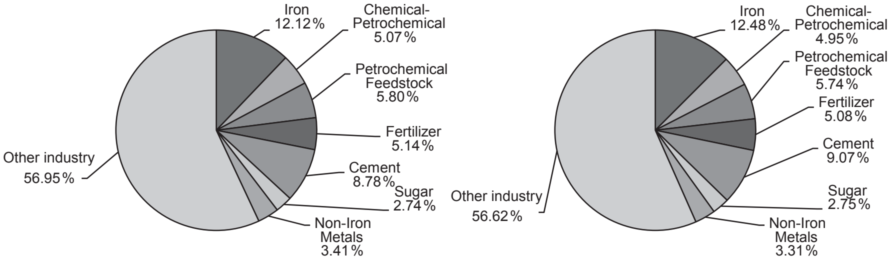


Fig. 1.18 Energy/exergy flows at sectoral level of a geopolitical region



a Primary energy consumption **b** Exergy associated to primary sources

Fig. 1.19 Energy and exergy consumption from primary sources in Turkey. (Data from [7])

lieved to take a larger share of transportation fuels. Among all transportation means, road transport is expected to evolve the fastest in the coming decades and to offer the most of exergetic improvement among all transportation ways. In [8] the energy and exergy efficiencies of the transportation sector for six countries are presented as shown in Fig. 1.20.

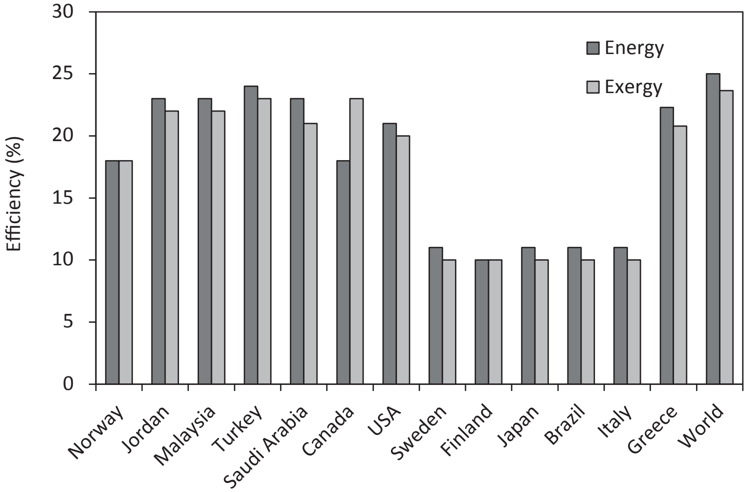


Fig. 1.20 Energy and exergy efficiency in transportation sector for six countries [8]

1.4 Sustainability Aspects

At the beginning of the twenty-first century, a new branch of science came out, namely the sustainability science, having an interdisciplinary character involving the following main disciplines: physics, chemistry, biology, medicine, social and economic sciences, and engineering. One of the goals of sustainability science is to model the complex interactions between society, economy, and environment, accounting also for resources depletion. One crucial aspect is the provision of theoretical foundations and tools for sustainability assessment.

Often in policy planning, indicators are used to assess a country or geopolitical region from various points of view: economic, social, etc. For example, the gross domestic product (GDP) is an economic indicator which indicates the well-being of a society. The aim of sustainability assessment indicators is to confer a basis for decision-making and policy elaboration toward sustainable development considering the integrated nature–society systems for a certain temporal perspective. In general, sustainability assessment indicators quantify in an integrative manner the economic, social, environmental, and institutional development of a country or region.

Table 1.4 gives some significant indicators for sustainability assessment. Certainly, the indicators have some degree of subjectivity because it is not actually possible to objectively determine and fully understand the interrelationships between social change and environment and economic development. The independent formulation of environmental, economic, and social indicators is more facile. For sustainability assessment, the developments in society, economy, and the environment are denoted as drivers. These developments (or changes) exert pressure on the sustainability, and as a consequence, the sustainability state changes in some direction. This eventually leads to foreseeable impact on sustainable development:

Table 1.4 Categories and kinds of indicators influencing the sustainability assessment

Kind / Category	Drivers indicators	State indicators	Responses indicators
Social	Unemployment rate	Poverty gap index	GDP on education
	Population growth rate	Income inequality index	Childhood immunization
	Adult literacy rate	School life expectancy	Infrastructure expenditure per capita
	Motor fuel consumption per capita	House price per income	Health expenditure per capita
	Loss rate due to natural disasters	Floor area per person	Hazardous chemicals in foods
Economic	Per capita GDP	Proven mineral reserves	Environmental protection expenditure
	Investment share of GDP	Fossil fuel reserves	Funding rate on sustainable development
	Annual energy consumption	Lifetime of energy reserves	Amount of funds on sustainability
	Natural resource consumption	Share of renewable energy	Percentage of new funds on sustainability
	Capital goods imports	Manufacturing added value	Funding grants on technology
Environmental	Water consumption per capita	Groundwater reserves	Wastewater treatment expenditures
	Generation of wastes	Monthly rainfall index	Natural resource management
	ODP substances emission	Desertification rate	Air pollution mitigation expenditures
	Emission of GHG, SO_2, NOx	Pollutants concentration	Waste management expenditures
	Energy use in agriculture	Acute poisoning	Number of restricted chemicals
Institutional		Scientists number per capita	Policy on sustainable development
		Engineers number per capita	Environment protection programs
		Internet access per capita	GDP share of R&D expenditures
		Telephone line access	Number of R&D personnel per capita
		Other information channels	Ratification/ Implementation of agreements

It improves or degrades the sustainability. The society can respond to this by taking actions to change the impacts directly (see the double arrow in the figure). In addition, the society can send feedback to drivers (i.e., to impose educated changes

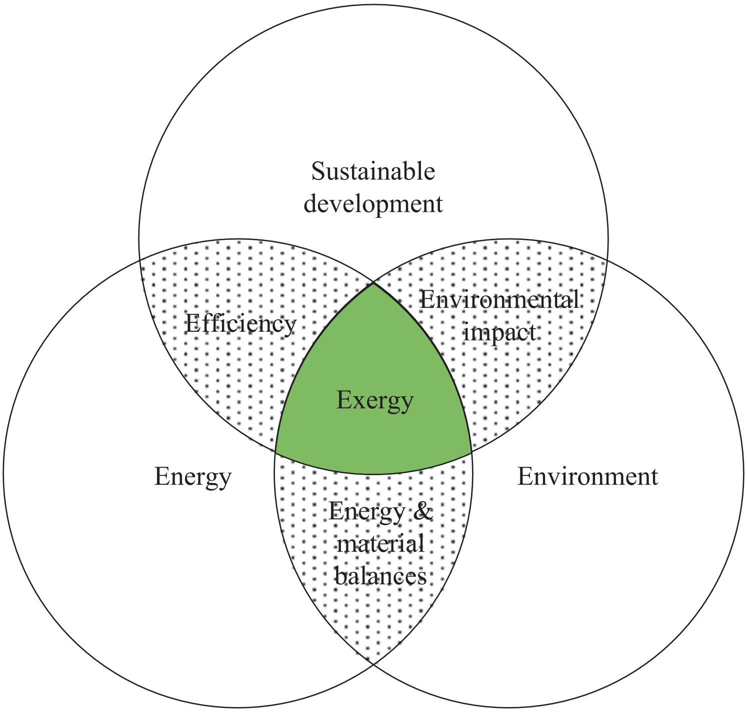


Fig. 1.21 Representation of the exergy at the confluence of energy, environment, and sustainable development

in the society, economy, environment). The responses can also act directly on the pressures and on the state of sustainability by applying adequate measures if possible. The responses must be effective, because their effectiveness affects directly the sustainable development. For sustainability assessment, this model simplifies to drivers–state–responses (DSR) or pressure–state–response (PSR).

Some specific aspects on elaboration and adoption of some holistic sustainability assessment methods are discussed as follows and shown in terms of their general confluence in Fig. 1.21:

- Sustainability assessment should integrate ecological conditions' assessment of human and life systems' habitat with economic development, social well-being, and with equity and disparity of current population and future generations.
- Obtain a consensus on adoption of a time horizon sufficiently long to be in accordance with ecosystem timescale and anticipated society timescale.
- Sustainability indicators and indices must be able to link sustainability categories to society goals.
- Sustainability assessment should integrate the following category of models:
  - Economic models
  - Stress–response models

  - Multiple capital models
  - Social–economic–environmental models
  - Human–ecosystem well-being models
- Definition of a reference environment (or state) is required for determining the sustainability change.
- Monetary assessment of environmental damage should be included in sustainability assessment.

The practical connection between wasted exergy and environmental impact can be discovered by correlating recorded emission data at the level of a region or globally with the chemical exergy of emitted pollutants. Here, some exergy destructions versus emission data are, as correlated, presented for Ontario, as a relevant example. The general aspects of environmental policy in Ontario can be described as follows:

- In Ontario, an Environmental Protection Act by the Ministry of Environment exists giving the legislation on environmental quality and air pollution limits which are conceived such that human health and the ecosystem are not endangered.
- The potential of a substance to impact on the environment is evaluated using a set of ten parameters:
  - Transport
  - Persistence
  - Bioaccumulation
  - Acute lethality
  - Sublethal effects on mammals
  - Sublethal effects on plants
  - Sublethal effects on non-mammalian animals
  - Teratogenicity
  - Mutagenicity/genotoxictiy
  - Carcinogenicity
- An aggregated indicator is determined based on the ten impact parameters (above), referred as the point of impingement (PoI) which is determined based on the best known available pollution control technology.
- The methodology denoted removal pollution costs (RPCs) is applied to correlate the exergy of the waste stream with the cost of removing pollutants from the waste stream prior to discharge into the surroundings. The cost of waste emissions is evaluated as the total fuel cost per unit fuel exergy multiplied by the chemical exergy per unit fuel exergy, and divided by the exergy efficiency of the pollution removal process.
- In Canada, the environmental pollution costs (EPCs) are estimated based on qualitative and quantitative evaluations of the pollution cost to the society for compensation and correction of the environmental damage and to prevent harmful discharges into the environment. Table 1.5 gives the EPCs of Ontario pollutants.
- The average composition of VOC emissions in Ontario are approximated as given in Table 1.6.
- The average compositions of PM emissions in Ontario are given in Table 1.7.

Table 1.5 Estimations of exergetic cost of atmospheric pollutants in Ontario. (Sources: [10–13])

Pollutant	*EPC* (\$/kg)	*M* (kg/kmol)	*MEPC* (\$/kmol)	ex^{ch} (MJ/kmol)	ex^{PC} (\$/MJ)	*PoI* (μg/m^3_{air})
CO_2	0.0402	44	1.77	19.60	0.090	56,764
CH_4	1.2998	16	20.80	831.66	0.025	N/A
NO_x	3.8944	38	148.18	72.4	2.047	500
SO_2	3.551	64	227.26	310.99	0.731	830
CO	5.5074	28	154.21	275.00	0.561	6000
VOCs	0.603	44	26.53	1233.00	0.021	N/A
PM	5.5074	68	374.50	436.00	0.860	N/A

Costs are in \$ 2013 based on the Canadian consumer price index

Table 1.6 Approximated average VOC composition and characteristics in Ontario. (Sources: [11, 13])

VOCs	Formula	*M* (kg/kmol)	T_0 (kmol/kmol)	ex^{ch} (MJ/kmol)	*PoI* (μg/m^3_{air})
Methanol	CH_3OH	32	0.020	612	12,000
Acetonitrile	CH_3CN	41	0.823	1169	180
Acetaldehyde	CH_3CHO	44	0.001	1063	500
Acetone	CH_3COCH	58	0.111	1636	48,000
Acetic acid	CH_3COOH	60	0.025	780	2500
Butanone	$C_2H_5COCH_3$	72	0.015	2755	250
Toluene	$C_6H_5CH_3$	92	0.005	3771	2000

Table 1.7 Approximated average PM composition and characteristics in Ontario. (Sources: [12, 13])

PM	Formula	*M* (kg/kmol)	*y* (kmol/kmol)	ex^{ch} (MJ/kmol)	*PoI* (μg/m^3_{air})
Lead	Pb	207	0.053	249.2	10
Cadmium	Cd	112	0.097	298.4	5
Nickel	Ni	59	0.185	242.6	5
Chromium	Cr	52	0.210	584.4	5
Copper	Cu	63	0.173	132.6	100
Manganese	Mn	55	3.115E-7	487.7	7.5
Vanadium	V	51	0.214	721.3	5
Aluminum	Al	27	0.006	795.7	26
Calcium	Ca	40	0.054	729.1	14
Magnesium	Mg	24	0.008	626.9	60

- The fuel cost for three types of fossil fuels, namely coal, no. 6 fuel oil, and natural gas, are in average value of CN\$2013 as follows:
  - Average coal: \$1.411/GJ LHV
  - Average no. 6 fuel oil: \$1.864/GJ LHV
  - Average natural gas: \$3.899/GJ LHV
- Table 1.8 gives the EPC and RPC values for the main fossil fuels in Ontario.

Table 1.8 Environmental pollution costs *(EPCs)* and removal pollution costs *(RPCs)* for fuels. (Source: [14])

Pollutant	*EPC* ($/GJ$_{\text{fuel exergy}}$)			*RPC* ($/GJ$_{\text{fuel exergy}}$)		
	Coal	No. 6 fuel oil	Natural gas	Coal	No. 6 fuel oil	Natural gas
CO_2	5.2662	5.7352	7.7184	3.35	2.7604	1.7822
CH_4	5.1724	1.1524	0	0.8174	0.1608	0
NOx	0.0469	0.03082	0.03082	0.938	0.469	0.3886
CO	2.1038	0.03082	0.3484	7.5442	0.0938	0.4556
SO_2	0.4958	0.402	0	2.5594	1.5544	0

Monetary values are in CN$ 2013. The data are for Ontario

A simplified method to estimate the cost of pollutant removal from the waste stream is based on the exergy efficiency of pollutants removal. According to [14], this exergy efficiency is in the range of 1–5 %. Therefore, once the exergy destroyed due to pollutant discharge is known, the required exergy to remove the pollutant from the waste stream can be calculated. Furthermore, the average price of exergy can be estimated for any geopolitical region; for Canada, it is approximated $C_{ex}=8.4$ ¢/kWh = 2.3 ¢/MJ. When the exergy required to remove the pollutants is multiplied with exergy price, the removal pollutant cost is obtained. Therefore, one has

$$RPC = C_{ex}\psi_{pr}Ex_{d,pw} \tag{1.5}$$

where C_{ex} is the exergy price, ψ_{pr} is the exergy efficiency of pollutant removal from the waste stream, and $Ex_{d,pw}$ is the exergy destroyed due to pollutant waste in the environment.

Assuming an average exergy efficiency of pollutant removal from waste stream of 3 %, the *RPC* can be estimated as 0.7$/GJ. The removal pollution cost of power generation can be roughly estimated based on statistical data that allow for the estimation of the exergy destructions. Table 1.9 gives the rough estimate of *RPC* associated with Canadian power generation. As given, the total *RPC* for power generation

Table 1.9 Removal pollution cost at power generation in Canada. (Source: [8])

Primary energy	Exergy input (PJ)	Power output (PJ)	Exergy destruction (PJ)	*RPC* (M$)	ψ_{pr} (%)
Nuclear	1073	339	734	514	32
Hydro	1698	1358	340	238	80
Coal	630	378	252	176	60
Fuel oil	62.5	23	39.5	28	37
Natural gas	254	112	142	99	44
Natural gas liquids	33.6	8	25.6	20	24
Diesel fuel	8.3	3.2	5.1	4	38
Biomass	66	19	47	33	29
Secondary sources	1629	543	1086	760	33
Overall	5454	2783	2671	1870	51

Table 1.10 Life cycle emissions into the atmosphere for power generation technologies (kg/GJ) (Source: [10])

Technology	kg per GJ fuel exergy							
	CO_2	CH_4	NO_x	SO_2	CO	VOCs	PM	
Coal-fired power plants	274	73	0.180	0.400	1.374	0.251	8.463E-6	
Fuel oil-fired power plants	176	47	0.115	0.200	0.876	0.160	5.439E-6	
Natural gas-fired power plants	112	30	0.073	0.150	0.558	0.102	2.557E-6	
PV power generation	44	12	0.045	0.090	0.038	0.003	1.336E-6	
Wind power generation	33	9	0.033	0.070	0.028	0.003	1.024E-6	
Hydro power	9	2	0.006	0.015	0.044	0.008	0.268E-6	
Nuclear power generation	48	13	0.032	0.065	0.241	0.044	1.488E-6	
Canada averages								
	CO_2	CH_4	NO_x	SO_2	CO	VOCs	PM	Total ($/MWh)
kg pollutant per MWh power	42	11	0.029	0.060	0.194	0.035	1.288E-6	
EPC_{ex} ($ per MWh power)	1.7	14.7	0.1	0.2	1.1	0.02	7.1E-6	17.8

EPC_{ex} exergetic environmental pollution cost

is ~1870 M$ and the overall exergy efficiency of the power generation sector is 51 %. The removal pollution cost becomes $2.5/MWh generated power.

Life cycle pollutant emission from power generation technologies is given in Table 1.10 based on multiple literature data sources as follows: [10–14]. Amounts of atmospheric pollutant are given with respect to the GJ of source exergy. Using the data from Table 1.8, weighted average pollutant emissions are obtained for the Canadian power generation mix. The averages are given in kilogram of pollutant per MWh of power generated; in order to convert from source exergy basis to generated power basis, the average Canadian exergy efficiency of power generation is used. Then, the exergy-based environmental pollution cost for power generation is calculated for each pollutant in $/MWh; the Canadian average of EPC_{ex} is $17.8/MWh; therefore, the cost of pollutant removal from the waste stream is much lower to the society than the cost of pollutant emission.

Note that materials used for system construction bring associated embodied energy and pollution. The cost of pollution associated with the construction of power generation facilities, reparations, and maintenance is not included in the results shown in Table 1.10. Table 1.11 gives the embodied energy and pollution amount and cost with various construction materials relevant to drying systems. Concrete, copper, and fiberglass bring the highest among the environmental pollution cost of the listed materials. The highest embodied energy is due to aluminum fabrication, which, as it is known, requires an energy-intensive electrochemical process.

Table 1.11 Embodied energy, pollution, and EPC in construction materials. (Source: [14])

Material	*EE* (GJ/t)	*SE* (kgCO$_2$/GJ)	EPC_{ex} (\$$_{2013}$/GJ)
Concrete	1.4	24	70.5
Iron	23.5	11	29.3
Steel	34.4	11	29.3
Stainless steel	53	62	29.3
Aluminum	201.4	10	29.9
Copper	131	57	60.1
Fiberglass	13	62	66.0

EE embodied energy, *SE* specific GHG emissions, EPC_{ex} exergetic environmental pollution cost

Using the concepts introduced here, the exergy destruction can be utilized to determine the environmental impact of a drying system in various manners as follows:

- The removal of pollution cost can be approximated by multiplying the exergy destruction with the exergy price estimated for a specific region or country.
- The rate of exergy input into the drying system can be used to determine the system physical size.
- From the system physical size, the mass amounts of materials required for system construction are determined.
- The amount of each construction material correlates with embedded energy required for its extraction and with GHG emissions and environmental pollution cost (see Table 1.10).
- The life cycle total exergy input into the system is equal to the exergy required for system construction, system operation, and system salvage.
- Based on the life cycle total exergy input and the exergy efficiency of power and heat generation system, the exergy destruction can be determined at power and heat generation.
- The emissions and environmental pollution cost due to life cycle total exergy supply are determined based on the exergy destruction and exergetic environmental pollution cost of the power and heat generation subsystem.
- The exergy destruction of the drying system itself allows for the determination of pollutant wastes and environmental pollution cost for operation during the entire lifetime.
- If a percent of materials' recycling is provided, then the wasted energy and emissions of scrapped system can be determined.
- The total pollutant emissions and environmental pollution cost result from the summation of the terms associated with power and heat generation from primary sources, system manufacturing, system operation, and system scraping.

1.5 Fuels

Fuels are very important for society. Most of the fuels are used in combustion processes. A combustion process represents in fact a reaction of oxidation which is of thermochemical nature and occurs with the production of a flame. In this process, a fuel is combined with air from the atmosphere. It required certain activation energy to initiate the oxidation reaction. Typically, the activation energy is obtained by increasing the temperature of the combustion reactants (fuel and air). Electrochemical "combustion" process—more accurately denoted as electrochemical fuel oxidation—is used in devices such as fuel cells to generate electric power directly. Natural gas is the preferred fuel for solid oxide fuel cells—a commercially available technology to generate power and high-grade heat. Hydrogen is the preferred fuel for proton exchange fuel cells—also a commercially available technology to generate power and, possibly, to recover low-grade heat.

Avoidance of flame combustion is advantageous in many instances because it limits the number of side products of the reaction process, it allows for better heat recovery from product gases, and it may facilitate the separation of carbon dioxide. Some advanced technologies of combustion which operate flameless are catalytic combustion and chemical looping combustion. Regardless of the types of combustion technology, fuels that contain carbon atoms in their constituency generate carbon dioxide when reacting with air. If the source of fuel is any underground deposit such as oil well, coal mine, natural gas field, tar sand bitumen, and oil shale, then, by using such fuels in combustion process, additional carbon dioxide is released in the atmosphere, and this fact may have negative consequence on the environment as it affects the radiative balance of earth and it contributes to the global warming effect.

Fossil fuels are those fuels that can be mined from underground (undersea) deposits and include high percentages of carbon. The main types of fossil fuels are coal, petroleum, and natural gas. The common theories consider that fossil fuels are formed from fossilized life systems including any kind of vegetation and animal residuals which are buried since historical times and decomposed biochemically by processes such as anaerobic digestion.

There is an increased trend to promote alternatives to fossil fuels which are more environmentally benign. The leading candidate as alternative fuel is the hydrogen which is a carbon-free fuel and can be produced from sustainable energy sources such as renewables and nuclear, or from waste energy and materials. Other major fuel or fuel source—which is carbon-neutral—is the biomass. According to the definition, *biomass* represents the biological material of any recently living organism. Biomass has relatively rich energy content and can be converted to heat and electricity in multiple ways: thermally, chemically, electrochemically, photochemically, and biochemically. Not only that biofuels are better from environmental standpoint than fossil fuels, but in some cases they are also more effective. For example, biodiesel—which is derived from plants—has a higher cetane rating than the usual fossil-based diesel.

Fuels can be categorized into two major classes as fossil fuels and alternatives to fossil fuels. Figure 1.22 illustrates a general classification of fuels. It is shown that conventional fossil fuels are coal, petroleum (oil), and natural gas as well as al petrochemical fuels obtained in refineries such as gasoline, diesel, and refined natural gas. There are some unconventional fossil fuel sources which started to be exploited more recently. These sources include tar sand bitumen, oil shale, and gas hydrates

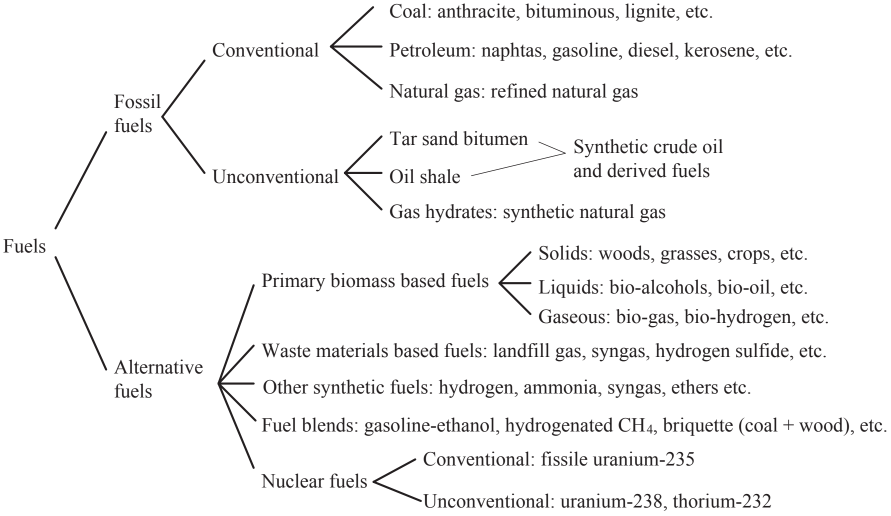


Fig. 1.22 Classification of fuels

deposits. Synthetic crude oil and synthetic natural gas can be obtained from unconventional fossil fuel sources which can be further processed to obtain end user fuels.

As indicated in the figure, the first and the major alternative to fossil fuels is the biomass. This is a very diverse source of fuels containing organic substances, derived from recently lived biological systems. Rough biomass can be combusted directly, or it can be processed to obtain higher quality fuels as solids, liquids, and gases. Waste materials and recovered waste energy can be also used to produce fuels. Some technologies of waste recycling to fuels are presently studied worldwide, for example, conversion of waste plastic materials to diesel fuel. Hydrogen is also an alternative fuel if it is derived from sustainable sources and by using sustainable technologies with limited or no environmental pollution. Other synthetic fuels may be ammonia, urea, ethers, etc. Another alternative to fossil fuels is represented by fuel blends. Fuel blends emit lower carbon per unit of released energy because a part of emissions originates from a biofuel such as bioethanol, while another part is derived from fossil fuel component.

Calorific value represents the essential technical parameter of a fuel which expresses the heat which can be released per quantity of fuel utilized. Here, the quantity of fuel can be generally measured in kilogram, but other units are also used depending on the nature of the fuel. For fluids, the quantity is typically measured in volume units such as barrels (for petroleum) or normal cubic meters (for natural gas). The calorific value of fuels is usually given in one of the following two forms:

- Gross calorific value (GCV) of solid fuels or higher heating value (HHV) for fluid fuels which represents the heat of combustion in the case when all combustion products are brought to the reactants' (fuel and oxidant) temperature, condensing all water vapor. Note that the gross heating value accounts for water

Table 1.12 Reaction enthalpy at carbon, hydrogen, and sulfur oxidation

Element	Oxidation reaction	Reaction enthalpy			Remark
		kJ/mol	kJ/kg	kJ/dm^3	
Carbon	$C + O_2 \rightarrow CO_2$	−393,486	32,790	68,580	Amorphous C at room temperature
Hydrogen	$H_2 + 0.5O_2 \rightarrow H_2O$	−241,811	120,905	9957	Standard pressure and temperature
Sulfur	$S + O_2 \rightarrow SO_2$	−296,792	9275	18,179	Beta phase at room temperature

existent in the fuel prior to combustion, in case that is of relevance for solid fuels such as coals and biomasses.

- Net calorific value (NCV) of solid fuels or lower heating value (LHV) of fluid fuels which represents the heat of combustion in the case when all products are brought to the reactants' temperature but water remains in vapor phase; the NCV (LHV) is determined by subtracting the heat of evaporation of water from GCV (HHV).

Fuels release energy due to the exothermic oxidation reaction with atmospheric air. Three atomic elements included in the molecular structure of any fuel are responsible of heat generation by oxidation, namely carbon, hydrogen, and sulfur. The heat released during oxidation of carbon, hydrogen, and sulfur is equivalent to the formation enthalpy of carbon dioxide, water, and sulfur dioxide. The oxidation reactions are detailed in Table 1.12. It can be observed that carbon has the highest reaction oxidation enthalpy per unit of volume, while hydrogen has the highest oxidation enthalpy per unit of mass.

In general, if a fuel is in contact with atmospheric air it does not ignite. The activation energy required for the initiation of a combustion process can be obtained by increasing the fuel temperature. In a standard atmosphere (defined by 21 % molar fraction of oxygen and a total pressure of 101.325 kPa), the lowest fuel temperature at which combustion is initiated without any energy from exterior such as a flame or a spark is termed as *autoignition temperature* (AIT). Simplified kinetic models are usually elaborated to predict AIT. The model must assume an air–fuel mixture at certain temperature, and based on mass and energy balance equations and chemical kinetics equations, a mathematical system of equation is formulated and solved in a transient mode to predict the evolution of species concentrations in time. If temperature is lower than AIT, the mixture is stable at chemical equilibrium. If the temperature is equal or higher than AIT, then the forward reaction proceeds at high enough rate to produce autoignition.

In order for solid and liquid fuel to combust with air, a mixture has to be created between fuel vapors and ambient air (oxygen). A nongaseous fuel can emanate vapors due to evaporation or sublimation effect at the liquid–gas or solid–gas interface, depending on the case. Vapor generation is influenced by the pressure and temperature conditions. At standard pressure, the minimum temperature at which sufficient vapor is generated at the surface vicinity to form a flammable mixture with atmospheric air is denoted as *flash point temperature* (FPT). A source of ignition is required to inflate the flammable mixture formed at FPT. The FPT is a very important safety parameter of a fuel because it indicates the presence of combustible vapor and flammable mixtures of gases.

Ignition of any fuel can be initiated only in specific conditions of temperature, pressure, and oxidant (air) concentration. In atmospheric air, at standard pressure and temperature (101.325 kPa and 298.15 K), the fuel must be at a temperature higher than FPT (see above), but in addition, the vapor concentration must be in a specified range denoted as *flammability limits*. The *lower flammability limit* (LFL) is defined as the volumetric concentration of vapor fuel in air below which there will be not enough fuel to allow for combustion to be self-sustained. If fuel concentration is too high, then another factor limits the ignition process: There is not enough oxygen for the combustion reaction to be maintained. The *upper flammability limit* (UFL) is defined as volumetric concentration of fuel vapor in atmospheric air over which there is not enough oxygen to sustain combustion in the vicinity of the ignition point. For a combustion flame to be maintained, the fuel vapor concentration must be between LFL and UFL.

As shown previously, liquid fuels are the most important for transportation applications; they are petroleum-derived fuels. The word “petroleum” comes from Latin and is a combination of two words: “petra” which means rock and “oleum” means oil. Therefore, petroleum is a designation for “oil found in rocks (sediments).” Petroleum is a mineral resource comprising a range of hydrocarbon-based oils which can exist in an underground (or undersea) rock deposit as liquids, gases, or solids. Similarly as coals—according to widely accepted theory—petroleum is formed from fossilized biological matter containing mostly lipids, amino acids, carbohydrates, and lignin.

Petroleum is a mixture of hydrocarbons that range from light ones (carbon number lower than five: methane, ethane, propane, butane, pentane) to heavier ones such as paraffin. Petroleum is toxic and flammable, and apart from carbon (83–87 %) and hydrogen (10–14 %), it comprises sulfur (0.5−6 %) and some metals. There is a large variety of petroleum reservoirs throughout the world—both conventional and nonconventional—such as oil fields, natural gas fields, coal bed methane, oil shale, and tar sand bitumen reserves. In this section, we refer to main categories of conventional petroleum sources (crude oil, natural gas, oil shale, and tar sand bitumen) and to their properties.

The main resource extracted from a conventional oil field is crude oil consisting of a complex mixture of polymeric hydrocarbon chains of two categories: volatiles and resins. The lighter (low molecular mass) fractions—volatiles may be of naphthenic, aromatic, paraffinic, or combined nature. The more condense (heavier) fractions of hydrocarbons in crude oil consists of waxes and asphaltenes. Crude oil may also contain sulfur, nitrogen, oxygen, metals, and other elements in some smaller fractions.

One of the precursors of crude oil is “kerogen” which is a mixture of organic compounds and has a molecular weight of the order of 1000 kg/kmol. Different kerogens can release other fossil fuels such as natural gas, shale, or bitumen from

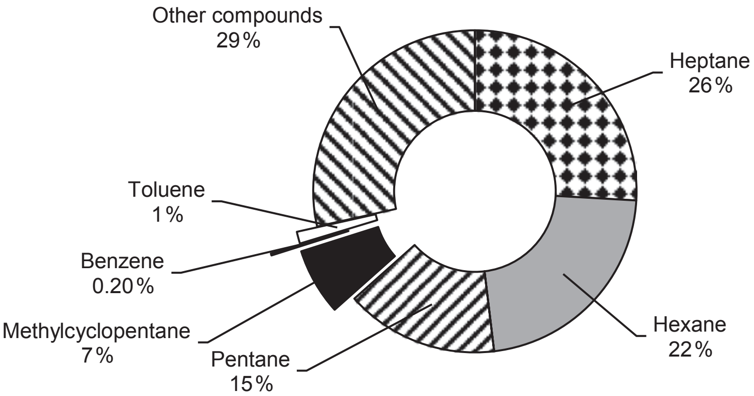


Fig. 1.23 Typical composition of crude oil. (Data from [15])

tar sands. Bitumen represents the fraction of kerogen which is soluble in organic solvents. The conversion of kerogen into fossil hydrocarbons is referred to as catagenesis.

Naphtenes are cycloalkanes—a class of saturated hydrocarbons having at least one ring of carbon atoms in their molecular structure, having the chemical formula $C_nH_{2n-2r+2}$, where $r > 1$ represents the number of carbon rings. Aromatics are some special types of hydrocarbons such as toluene, xylene, and benzene which produce polymers and have a planar molecular structure with at least one carbon ring and $4n+2$ electrons contributing to the covalent bonds. Waxes are polymerized hydrocarbons that are soluble in organic solvents and insoluble in water. They are of plastic aspect and are solid state at 25 °C, although their melting point is very low (slightly above ~40 °C). Asphaltenes consist of a mixture of chemical compounds including hydrocarbons, nitrogen, oxygen, sulfur, and metals with a carbon-to-hydrogen atomic ratio of approximately 0.8 and molecular mass of 800 kg/mol on average.

Figure 1.23 presents the main volume fraction of various components in a typical crude oil composition. Pentane includes at least three molecular variations as n-pentane, isopentane, and cyclopentane. Also, both n- and isostructures are included in the diagram for hexane and pentane, respectively; and in addition, cyclohexane is accounted for in the diagram from the figure, under the general label "hexane."

There are no (or very few) applications where crude oil is used directly because of its low calorific value, water content, metals, and pollutants which may affect negatively any king of combustion facility (or other types of devices that may use crude oil). Crude oil has low calorific value in its original state and has no practical applications. This is why, crude oil and all other forms of petroleum must be refined and converted to petrochemical fuels which become valuable commodities. Examples of petrochemical fuels are liquefied petroleum gas (LPG), kerosene, diesel, gasoline, jet fuels, and others. Note that a refinery also produces other valuable products such as waxes, asphalts, plastic materials, lubricants, and greases.

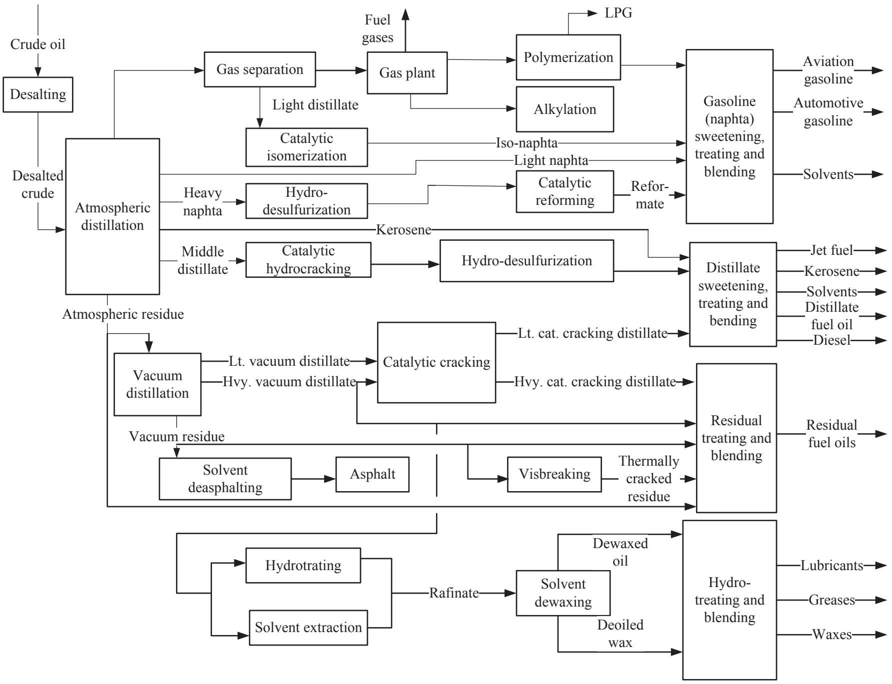


Fig. 1.24 Simplified diagram of a petrochemical refinery

Even after the separation of water, hydrogen sulfide, and other components, crude oil is still a mixture of many hydrocarbons ranging from very light to very heavy components. In a refinery, the crude oil has to go through successive chemical and physical processes such as desalination and cleaning, distillation, hydrotreating, etc. Distillation separates crude oil into different fractions depending on the difference of boiling temperatures. Atmospheric distillation is applied to separate the light compounds, whereas vacuum distillation extracts the heavier fuels.

Figure 1.24 illustrates a simplified diagram of a petrochemical refinery indicating the main fuel and non-fuel products. Some of the main components of the diagram are the distillation columns, the crude oil furnace, various catalytic reactors, separators and heat exchanger network, visbreaking unit, and solvent dewaxing unit.

Crude oil is heated initially to 350–380 °C and vaporized thus in proportion of 75 % and then distilled at a pressure of about 200 kPa; the remaining 25 % atmospheric residue (liquid) is drawn at the bottom of the column. The flowing fuels result from the atmospheric distillation unit: heavy diesel, medium diesel, light diesel, and kerosene. The very light products, butane naphtha and the lighter ones, leave as vapor from the top of the column. The atmospheric overhead is partially condensed in heat exchangers. When they are cooled, the naphtha condenses and leaves as liquid, while the lighter products remain as gases. Uncondensed vapor flows to the fuel gas system, which is used as fuel for the furnaces.

The vacuum distillation unit operates at vacuum pressure (typically 18 kPa) to help in separating heavy hydrocarbons. The following products result from the vacuum distillation process: wash oil, heavy vacuum gas oil, and light vacuum gas oil. The residuum formed after the vacuum distillation process is eventually recovered as asphalt. The heavy vacuum distillate is partially converted in lubricants, greases, and waxes.

The range of petrochemical fuels obtained from crude oil refining is large and essentially listed as follows:

- Naphtha—with 5–7 carbon atoms in the molecule (used mainly as solvents).
- Gasoline—with 8–11 carbon atoms, which makes the basis of gasoline fuel for autos.
- Kerosene—with 12–15 carbon atoms, from which diesel fuel is extracted.
- Lubricating oils—with 16–19 carbon atoms; they show high normal boiling point.
- Solid hydrocarbons—with over 20 carbon atoms; they have melting point at higher values than ambient temperature and are classified in the order of increased molecular weight in paraffins, wax, tar, and asphaltic bitumen.

The fuel that is used mostly in road transportation is gasoline, which is a blend of aliphatic and aromatic chemicals obtained by the distillation of petroleum in refineries. Diesel fuel is also very common for road transport—especially for large capacity vehicles—and marine ships and rail locomotives.

Processing of petroleum to obtain diesel fuel is simpler with respect to gasoline. The important aspect in diesel processing regards reduction in sulfur content. The LPG is based mainly on propane, but often is mixed with butane in 60/40 proportion. The gases that compound LPG are all extracted from petroleum in refinery processes. The density of LPG is about the average of that of liquid propane and liquid butane at 25 °C. Alcohol-based fuels—such as ethanol and methanol—can be produced using petroleum as fossil fuel source. However, these fuels are mostly produced from biomass through fermentation and they are categorized here as alternative fuels.

Table 1.13 gives the properties of main petrochemical fuels. Regarding jet fuels, there are currently two main grades: Jet A-1 and Jet A, which are both kerosene-type fuels. There is another grade of jet fuel, Jet B, which is a wide cut kerosene (a mix of gasoline and kerosene), but it is rarely used, except in very cold climates. Jet A is a kerosene-based type of fuel, produced to an American Society for Testing and Materials (ASTM) specification and normally only available in North America. It has the same flash point as Jet A-1, but a higher freeze point (−40 °C). Jet B is a distillate covering the naphtha and kerosene fractions. It can be used as an alternative to Jet A-1. As it is more difficult to handle (higher flammability), there is only significant demand in very cold climates, where its better cold weather performance becomes important. In Table 1.13, in the row indicated "Jet Fuels," there are listed the average properties of Jet A and B fuels.

Table 1.13 Petroleum-derived fuels and their properties

Fuel name	Boiling point (°C)	Molecular weight (Kg/kmol)	Density (kg/m^3)	Carbon (%wt)	LHV (MJ/kg)	HHV (MJ/kg)	Chemical exergy (MJ/kg)	EF_H $\frac{kg_{co_2}}{GJ_{LHV}}$
Light naphtha	0–150	100–150	~750	83.7	44.9	48.1	44.5	68.2
Gasoline	35–200	114	~745	85.1	43.5	46.5	47.5	71.9
Heavy naphtha	150–205	150–215	~850	85.4	43.0	46.1	49.0	64.2
Diesel fuel	150–370	233	~747	85.6	42.8	45.8	44.2	73.3
LPG	−43	44	~580	81.8	46.0	52.0	54.9	65.3
Kerosene	205–260	170	~795	84.7	43.1	46.2	49.1	71.9
Jet fuel	156–293	185	~800	76.0	43.2	46.9	45.3	63.4
Fuel oil	260–425	>200	~990	85.4	40.1	42.9	41.4	78.1

LPG liquid petroleum gas (assimilated as propane)

1.6 The Transportation Sector

In any country, the transportation sector is characterized by intense energy demand. Figure 1.25 indicates the distribution of energy demand and GHG emissions for the transportation sector in Canada where the transportation sector accounts for about 32 % energy demand and 35 % GHG emissions. It can be observed that road transport is responsible for 78 % of GHG emissions in this sector. Figure 1.26 shows the fuel consumption in the Canadian transportation sector, as per fuel type. Motor gasoline is the major fuel in Canada; its consumption represents 54 % in energy terms from all fuels. Diesel fuel follows gasoline with 33 %, and next is aviation fuel with 10 %.

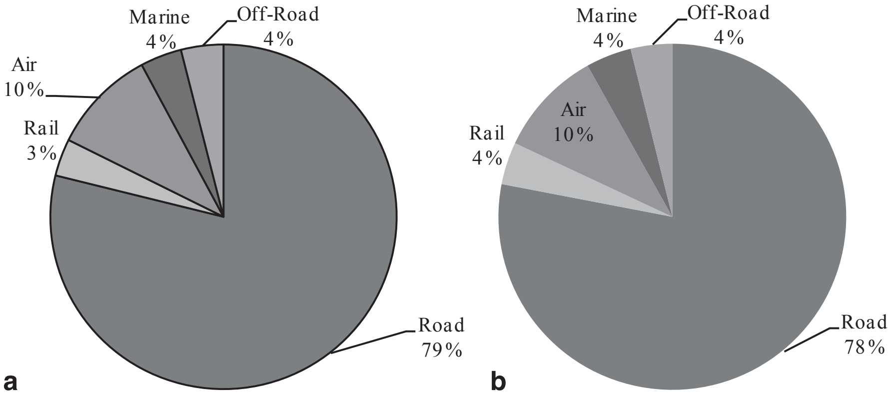


Fig. 1.25 Energy (**a**) and GHG emissions (**b**) by the transportation sector of Canada for each major transportation mode in 2008

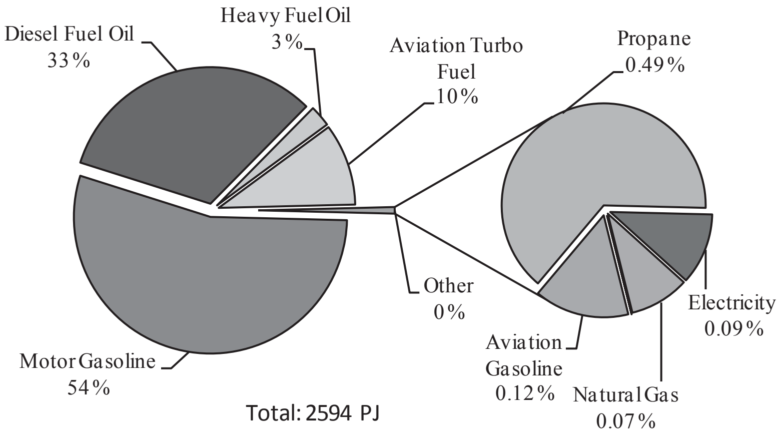


Fig. 1.26 Fuel consumption in Canadian transportation sectors, as per fuel type

Figure 1.27 details the energy and GHG emissions for all kinds of transport vehicles in Canada. According to these data, pollution is most due to passenger cars (25.3%) and heavy trucks (23.3%). It is expected that in the near future, the global demand for transportation of goods and people will significantly increase. If the transportation demand increases at the same pace with global population, the level of pollution will also rise significantly. In this section, the role of nuclear hydrogen for a cleaner and better transportation sector is studied.

Figure 1.28 compares the GHG emissions and air pollution indicators for hybrid, electric, fuel cell, and conventional passenger cars. The air pollution indicator quantifies the environmental impact of exhaust gases of automobiles other than GHGs, which include the following airborne pollutants: CO, NO_x, SO_x, and VOCs. Four real vehicles are considered: Toyota Corolla (conventional), Toyota Prius (hybrid), Toyota RAV4EV (electric), and Honda FCX (fuel cell). It is assumed that hydrogen is generated by grid electricity assuming average worldwide pollution indicators associated with electricity generation, namely 77.5 g GHGs per megajoule of electricity and 0.296 g/MJ as the air pollution indicator. All three alternative vehicle options reduce the lifecycle pollution to about half, with respect to a conventional vehicle. However, fuel cell vehicles show least air pollution among all, during the vehicle utilization stage. The electric vehicle is characterized by air pollution during the utilization stage mainly due to its battery recycling. If the GHG emissions of hydrogen production decrease, the fuel cell vehicle has the best likelihood to have the lowest carbon footprint.

Figure 1.29 provides a comparison of averted emissions based on different power sources, against distance travelled by trains annually. On the basis of the source energy, whether nuclear, Ontario Power Generation (OPG) mix in Ontario, Canada, or hydrogen from steam methane reforming (SMR), the utilization of heat rejected from thermal power plants, combined with hydrogen generated through a thermochemical Cu-Cl cycle and proton exchange membrane fuel cell (PEMFC) trains,

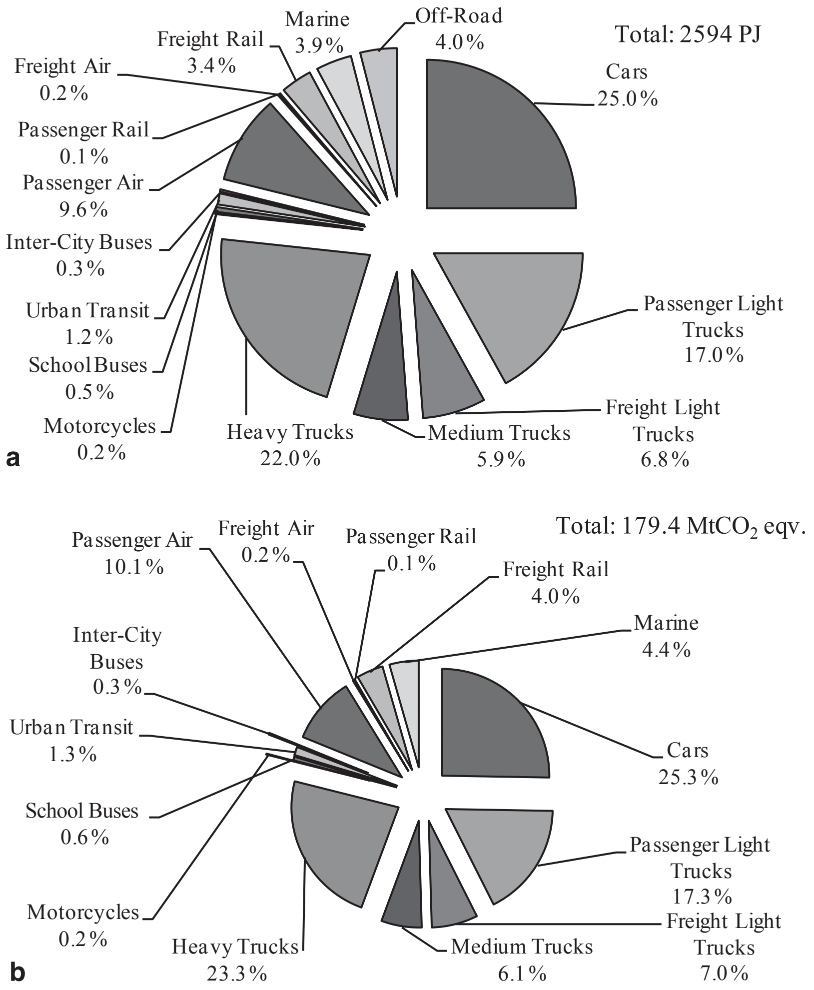


Fig. 1.27 Energy consumption (**a**) and GHG emissions (**b**) of transportation vehicles in Canada as per 2008 [16]

results in the lowest level of GHG emissions on the order of 0.10 kg/GJ. The higher efficiency of the PEMFC complements the performance of thermochemical hydrogen production, yielding the lowest GHG emissions at the prime mover, on the order of 0.04 kg/km (345 t by 2015 and 488 t by 2031). The actual impact of CO_2 emission reduction is significant when compared to the diesel alternative.

Table 1.14 shows detailed emission analysis of flight, landing, and takeoff for an Airbus A300 airplane at selected destinations departing from Toronto. As derived from the combustion equation, $C_{12}H_{23} + 17.75\ O_2 + 66.77\ N_2O_2 \rightarrow 12CO_2 + 11.5\ H_2O + 66.77\ N_2$, for complete stoichiometric combustion of 1 kg of kerosene, 3.4 kg of oxygen is needed, producing 3.16 kg of CO_2, 1.24 kg of water vapor, 1 g of NO_x, and 1–2.5 g

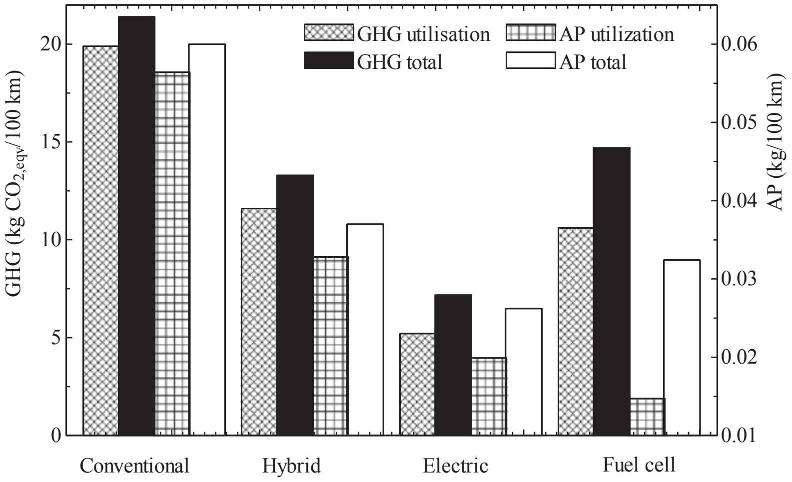


Fig. 1.28 GHG and air pollution (AP) related to the fuel utilization stages and total environmental impact for different types of vehicles

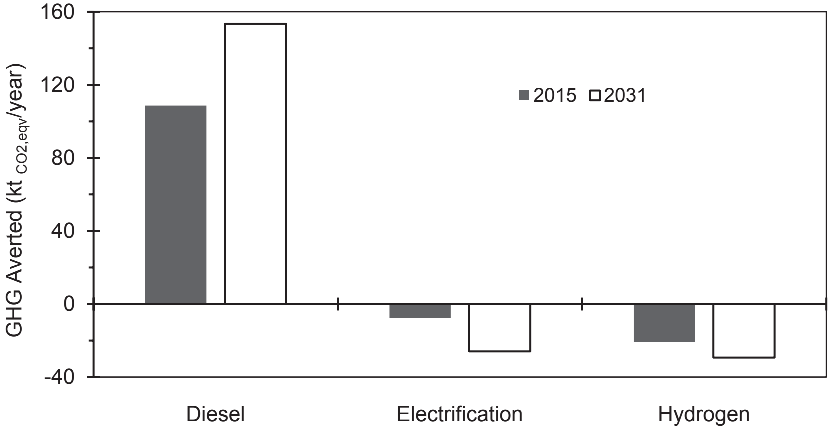


Fig. 1.29 Total equivalent GHGs averted by train transport

of CO. A typical passenger airplane consumes about 13,937 kg of kerosene (for a distance of 2716 km) for a trip from Toronto to Calgary.

1.7 Concluding Remarks

Combustion of fossil fuels appeared to be a sustainable activity during the industrial revolution. Then, the steam engine was invented and used in many fields of activity, including metallurgy and other industries. Beginning with 1700s, coal and biomass have been extensively combusted to generate pressurized steam to run engines

Table 1.14 Total emissions for an Airbus A300 airplane at selected destinations from Toronto

	Montreal	Calgary	London
Distance (km)	504	2716	5710
Fuel consumption (kg)	3677.3	13937.3	19005
Climb/cruise/descent (kg)	2875	13751.4	7553.7
Specific consumption (kg/km)	7.29	5.13	5.55
NO_x (kg) total	56.17	171.4	251.7
Climb/cruise/descent	45.29	171.5	214.0
HC (kg) total	2.43	4.19	5.10
Climb/cruise/descent	0.5	2.30	3.03
CO (kg) total	21.9	32.2	39.2
Climb/cruise/descent	3.1	10.25	12.74
GHG emissions (kg $CO_{2,eqv}$)	22.34	15.71	19.85

HC hydrocarbon emissions, *CO* carbon monoxide emissions, NO_x nitrogen oxide emissions

which were used to manufacture tools, equipment, railways, locomotives, etc., with increased productivity. Thus, this explains why the power of coal and burned wood seemed to be sustainable at that time and the evolution had been fast and straight forward. In twentieth century, petrochemical fuel became the dominant source of energy for transportation, although even today coal leads as a source of energy for power generation.

The steam engine revolution represented a crucial technological advance for the humankind, similar to that of mastering the fire. The steam engine, evolved into the combustion engine nowadays, allowed humans to generate power from much abundant resources than biomass, namely the petrochemical fuels (and other minerals, including nuclear).

However, the sustainability of the fossil fuel-driven heat engine technology gradually reduced until it became nearly unsustainable. This is mainly due to the fact that fossil fuel depletes. The technology as it is today must consume fuels for its own development; faster the world development is, faster is the depletion of the fossil fuel resources which support the technology. A second aspect is represented by the environmental imbalances caused by the industrial revolution. An extensive amount of carbon dioxide has been injected in the atmosphere in the last 150 years due to anthropogenic activity. It appears that the atmosphere—although being a vast reservoir—could not dump this accumulation and, from here, all the alarming effects such as the global warming, acid precipitation, ozone layer depletion, and other extreme events start.

One of the major consequences of the industrial revolution is the development of the railway transport. Synergistically, the railway transport accelerated the technology development within the industrial revolution era. The railway transport evolved from a steam engine locomotive-based system to the current technology based on electric-only and diesel-electric locomotives. Being part and consequence of the industrial revolution, the railway transport is subjected nowadays to the same sustainability concern as the energy production sector, that is, fuel depletion and environment pollution.

Chapter 2
Rail Transportation

2.1 Introduction

Transportation has been a critical issue to the humankind over the centuries, and it has shaped the past, is shaping the present, and will definitely shape the future. Human activities depend essentially on transportation; movement of goods and commodities, persons, and even communication via mail delivery services.

The sources of energy for propelling transportation activities vary throughout history, evolving in parallel with the development of communication systems. This relationship between transportation and communication has important social implications. The railway transport, in particular, is vital in times of crises, emergency situations, and when the military mobilization is necessary. The railway transport has the ability to provide redundancy during emergencies.

In antiquity, special systems were developed to transmit messages, strategic information, and goods within various jurisdictions. The postal transport within the Roman Empire employed the "cursus publicus," special walking couriers, who delivered messages between the postal mansions constructed 40 km apart from the main communication road. The same roads were used for land transport of larger goods by animal-pulled vehicles. This mode of land transport continued until the industrial revolution of the eighteenth century when the invention of steam engine and the rail transport gradually occurred. In its early development stages, rail transport was used in conjunction with mining operations, slowly reaching technological maturity by the mid-nineteenth century. The development of steam locomotive and the invention of the wrought iron rail technology were the two crucial factors that led to the establishment of the modern railway transportation.

The modes of rail transport are very diverse nowadays, as they involve complex operations and infrastructure. This chapter discusses the role of rail in transportation systems, its current status, and the opportunities for sustainable transportation solutions across the sector through clean rail development.

I. Dincer et al., *Clean Rail Transportation Options,* Green Energy and Technology,
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2.2 Rail Transportation Overview

Rail transport is employed to mainly carry passengers and goods (especially cargos), and can run on both single fixed-type and dual-type rails. It essentially covers light rail, heavy rail, and tram as well as funicular and monorail rail means. They provide numerous advantages, ranging from economic to social and energetic to environmental, which makes rail transport the best land transportation option for passengers and goods. It also appears to be the best public transportation option based on several criteria, such as number of passengers carried, congestion-free traffic, reduced amount of fuels and hence reduced amount of emissions per passenger, reduced cost, reduced road accidents, increased safety, increased speed, reduced use of land, better use of existing infrastructure, etc.

Rail transport has a well-established position among the transportation modes for passengers and freight. Figure 2.1 shows a classification of the passenger transportation modes. As well understood, transportation can be done on roads, air, rail, and sea. Passenger air transport differentiates two modes, namely scheduled and charter flight with the overwhelming majority of carriers being jet airplanes. Road transport is the most varied with respect to transportation means, starting from pedestrian, bicycle, motorcycle, automobile, and bus (coach). Rail transport vehicles for passengers can be categorized as: transit (commuter) trains, high-speed rail, and intercity rail, and also includes railcar on the streets in towns.

The maritime passenger transport is less used today due to its slow mode. The most used is the ferry transport, which actually can transport the pedestrians and passengers riding in all types of road vehicles. Cruise ship is mainly used for leisure transport. Figure 2.2 shows five types of freight transportation modes, namely, air, road, rail, maritime, and pipeline. As seen, the freight rail transport differentiates two modes, the unit train and carload. Furthermore, the rail, road, and maritime

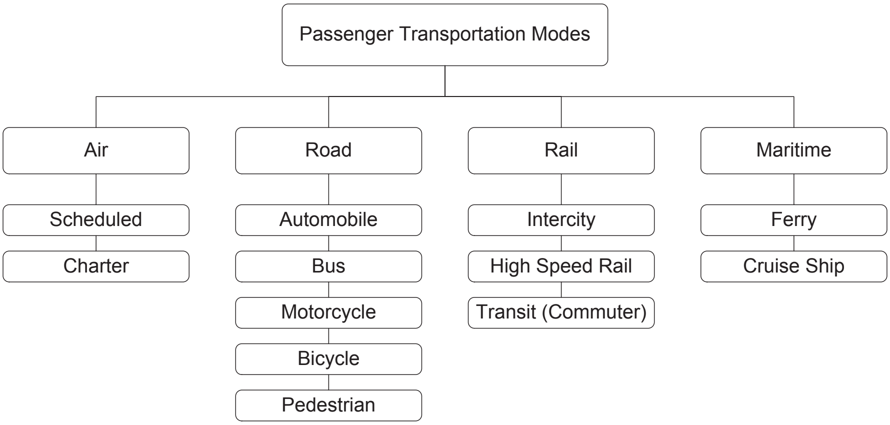

Fig. 2.1 Major passenger transportation modes. (Adapted from [17])

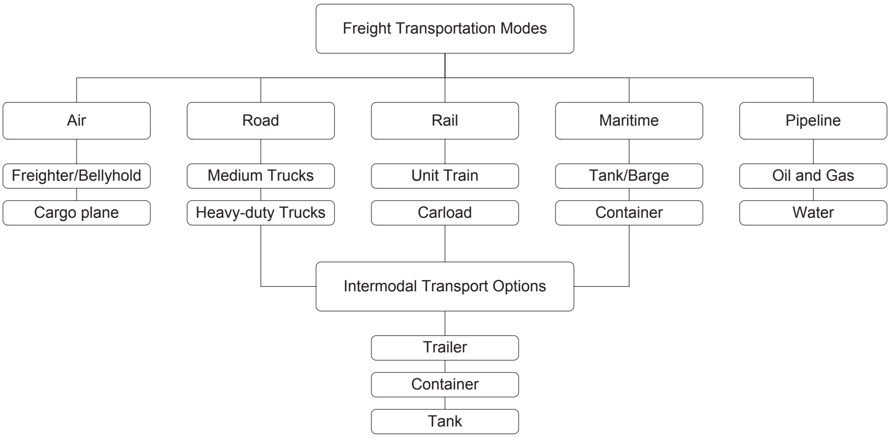

Fig. 2.2 Major freight transportation modes. (Adapted from [17])

transport integrated the unitary in the so-called intermodal transport. Three options are available for the intermodal transport: trailer, container, and tank.

Rail transport appears to be a widely used transportation mode in many countries. As a relevant example, in Germany, railway length is approximately 35,000 km, being the second largest in that country after the long-distance federal roads. Diesel is the primary fuel in North America for railway transport, while several countries, including European countries and Japan, use electricity as a primary source of energy for rail transport. Some developing countries, such as China and India, still use coal as the energy source. The energy consumption for rail transport is in-between the road truck transport and inland and coastal ship transport with approximately 400 kJ/t km.

When we look at the railway sector for the transport of passengers and goods, we observe an increasing use of this mode in almost every country due to the above-mentioned advantages, which may be generalized into four key benefits, namely, safety, rapidity, cost effectiveness, and environmentfriendliness. The growth in rail transport is expected to be doubled in the next decade by considering the economic growth in fast-developing countries, including China, India, and Turkey.

Several countries, such as Turkey, have developed strategic plans to go for speedy trains and started implementing their plans in a massive manner. The high-speed trains represent a complex development involving interdisciplinary aspects related to the prime mover development (with the use of high tech and advanced designs), rolling stock operations, traffic system and signaling, special rail infrastructure, commercial, and managerial issues.

In the subsequent paragraphs, some relevant information on high-speed trains is given, as summarized from Ref. [18]. The high-speed trains run at a speed of over 250 km/h, whereas the speed of conventional trains is limited to about 200 km/h. The high-speed trains currently in use can attain a speed of over 500 km/h; however, the practical maximum speed in operation is about 350 km/h. The braking distance from a speed of 350 km/h is of about 6.7 km.

It appears that high-speed train has the highest passenger-kilometer carried per unit of energy among all means of land transport. In addition, the land use for high-speed railway is three times smaller than land use of a motorway in terms of hectare per kilometer. Furthermore, all high-speed trains are electric trains operating with single phase current at 15–25 kV with typical frequencies of 50 Hz or 60 Hz. However, the construction and maintenance cost are relatively high. The capital cost of railway infrastructure is in average US$20 million per km with an annual maintenance of 0.5 % of the capital cost in railway. The specific capital cost on high-speed passenger trains is approximately US$80,000 per passenger seat, and typically a train has 350 seats. The train requires a maintenance cost of US$4 per km while it travels approximately 400,000 km/year.

The high-speed trains worldwide increased since 1964, when the first train was put in operation on the line between Osaka and Tokyo; growing from a few hundred kilometers, to 30,000 km in 2014 with prospects to reach over 40,000 km after 2025, with the rail operating up to 15 trains per hour. The high-speed trains are more effective for travels longer than 300 km, for which the actual travel time will be less than half when compared with the conventional transportation vehicles.

The freight railway transport represents the least costly alternative for massive, heavy, bulky commodities, and hazardous materials, being critical to the development of in-land industries. The reason for this fact is not only better energy efficiency and fuel economy of the rail transport with respect to truck transport, but also a better ability to carry massive products. According to the US statistics, the railway transport consumes less than 0.7 L of diesel fuel for 100 km to transport 1 tonne of freight [19]. In addition, the emission factors are better for the rail transport than for the trucking. As of today, if 10 % of the freight transported by road trucks are transported by rail freight, then 2.5 millions of carbon dioxide emissions would be mitigated [19].

Most hauled products of the rail freight transport include: grains, corn, soybean, corn syrup, ethanol, traffic control equipment, electro-mechanical equipment, machinery parts, HVAC equipment, lead-acid batteries, construction-related products (including railway pavement materials), drywall, paper products, aluminum, steel, sheet metal, structural steel, tubing, bars, steel profiles, studs, wood, glass, mirrors, office supplies and furniture, paints, solvents, detergents, cement, lime, aggregates and ready mix, automobile and truck repair parts, bottled water, specialty gases, and cars. Coal is the commodity that is mostly transported by the freight-rail. It follows farm products and non-metallic minerals, chemicals, and then food products.

There is a large variety of railcars for freight transport, namely, intermodal container on flat car, intermodal trailer on flat car, intermodal double stack, liquid-bulk tank car, open flat car, hopper car, box car, and cryo-car. Worldwide, an annual growth of few percent in the freight rail transport is remarkable.

It should be noted that the need for new locomotives has decreased by over 20 % during the past three decades due to the technological developments and improvements in locomotives and their systems. Such improvements and developments have helped to improve the overall efficiency by more than 25 %. There are even more potential integrated systems to improve the performance of the locomotives further and make them more efficient, cost effective, and environmentally benign. Such novel systems are described in detail in Chap. 6, and the case studies related to these integrated systems are presented in Chap. 8, based on various criteria, such as efficiency, cost and environmental impact.

2.3 Rail Transportation Infrastructure

Clean transport has been identified as a critical area of research in numerous countries, such as Canada, which aims to meet the mobility needs of the country and provide more efficient, more cost effective, and more environment- friendly transportation solutions to the people and goods, at the same time reducing the associated harmful effects on humans and other living species as well as the environment. In recent decades, there has been an overall improvement in the energy efficiency of transport in these countries as well.

To contextualize rail within the global transportation sector, it is important to first introduce the general characteristics of all transport systems, technical, operational, and commercial factors affecting the selection of a certain mode of transportation. Not only the locomotives and their design are important in the railway operation, but also the rail infrastructure, maintenance issues, and ownership (private or state owned companies). The railway system in North America operates as a unitary infrastructure as it allows for interchangeability and interoperability of line-haul locomotives and railcars everywhere across Canada, USA, and Mexico. In North America, the railroads are classified in three classes. If the railway carrier revenue is over US$250 million yearly (given in 1991 dollar indexed value), then the railroad is denoted as Class I. Some important Class I railways in North America are named here as:

- Union Pacific (UP) railway with more than 31,000 route miles and 8000 locomotives (major freight—fuels)
- Burlington Northern Santa Fe (BNSF) railroad with more than 32,000 route-miles and 7000 locomotives (major freight—consumer products)
- Canadian National (CN) railway with more than 22,000 route-miles
- Canadian Pacific Railway
- CSX Transportation (major freight—coal, coke, and iron)
- Norfolk Southern Railway (major freight—coal, coke, and iron)
- Kansas City Southern Railway
- VIA Rail (in Canada)
- Amtrack (in USA).

The railroads categorized under Class II are destined to freight transport of mid-sized revenue, greater than US$37 million per year but smaller than US$433 for

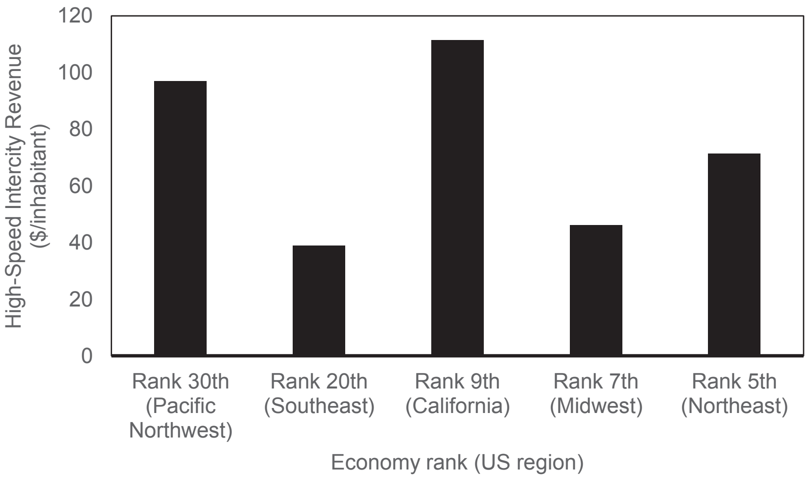

Fig. 2.3 A specific high-speed intercity revenue of railway operator correlated with the worldwide economy of the USA region. (Data from [19])

three consecutive years. The Class III railroads are of short distance with revenues less than US$20 million per year.

The freight-rail transportation in USA carries 16 % of the total freight tonnage representing 28 % of total tonne-km or approximately 6 % of the total freight which has been valued at US$600 billion in the year 2000 [19]. It is recognized that the freight-rail transport will enhance by 50 % by 2020 with respect to today. The average length for rail-freight transport is approximately 1000 km at a cargo cost, which is three times lower than for trucking. Regarding the passenger rail transport, this increased steadily during the years. The speed of intercity railway is of over 200 km/h in North America with more than 1500 track-km in USA. Figure 2.3 shows a correlation between the railway revenue for the high-speed intercity passenger transport in the USA and the rank of the economy.

The Canadian locomotive fleet is made up of nearly 3000 locomotives servicing the freight and passenger transportation operations (Table 2.1). Freight locomotives and operations make up the majority of rail operations, representing more than

Table 2.1 Canadian locomotive fleet for 2011. (Source: [20])

Locomotive fleet	2978
Freight operations	2731
Passenger operations	247
Diesel fueled	2933
EPA emission limit compliant	1433
Tier 0/0+	517/170
Tier1/1+	111/94
Tier 2	541

EPA Environmental Protection Agency

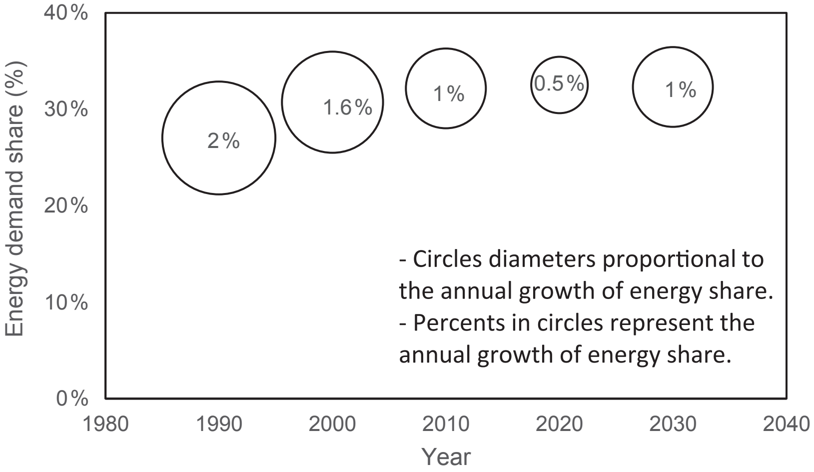

Fig. 2.4 Annual share of energy demand for transportation sector in Europe. (Historical records and predictions until 2030; data from [21])

90% of the Canadian locomotive fleet. The fleet is almost entirely of diesel-electric locomotives, operating with either two-stroke or four-stroke prime mover diesel engines that are coupled with an electric alternator/generator to convert shaft power to electric and power the traction motors and control systems.

The railway industry has a great growth potential. Major transportation corridors continue to develop. The capital expenditures were US$54 billion in the USA for the 1990 decade, of which 67% is infrastructure investment and the rest equipment. Although the capital expenditures with respect to revenue are four times higher than all manufacturing processes, the investment is safer [19]. Since the rail transportation sector is predicted to grow, the associated energy demand with this activity must increase. In Ref. [21], it is shown that not only energy but also the energy share of transportation sector in general with respect to other sectors of activity is predicted to steadily increase. This fact is illustrated graphically as shown in Fig. 2.4. The share of rail transport with respect to other transportation mode is predicted to be around 6.5% in Europe. However, the railroad transport is predicted to grow and double in every year until 2030, as shown in Fig. 2.5.

2.4 Rail Transportation Challenges

Projections of Canada's green house gas (GHG) emissions for 2020 based on current emission reduction strategies exceed the Copenhagen target level by more than 100 megatons (Fig. 2.6). Significant effort is necessary in order to close this gap. Fossil fuel combustion is the primary source of GHG emissions—approximately 75% of total GHG emissions [22]—mainly from stationary and transportation combustion sources.

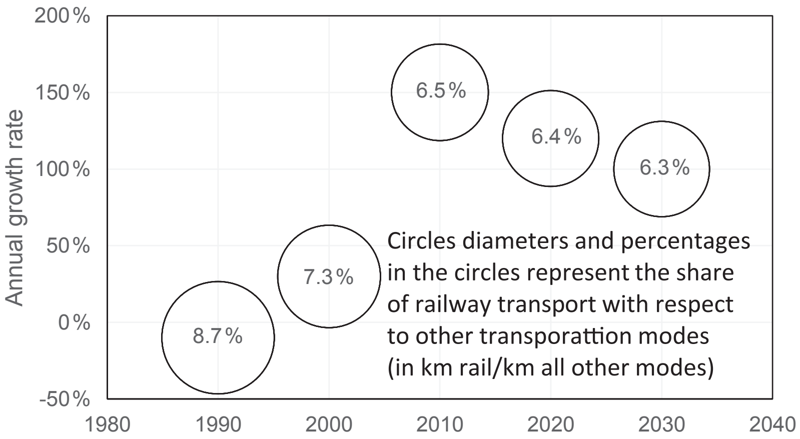

Fig. 2.5 Annual growth rate and the share of rail transport versus other transportation modes in Europe. (Data from [21])

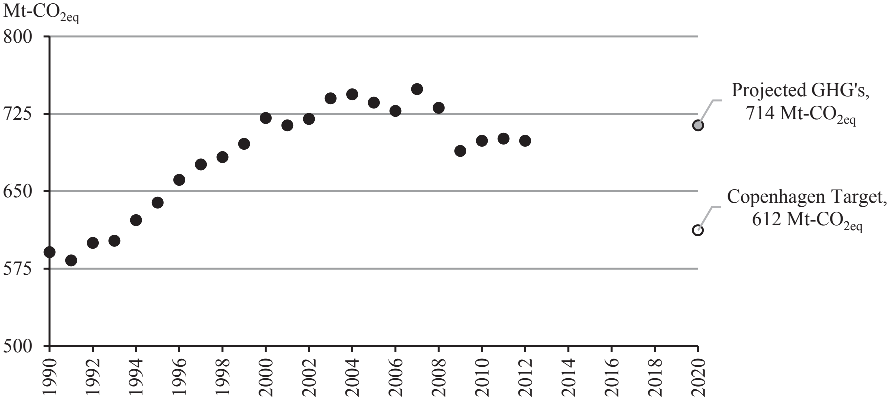

Fig. 2.6 Total GHG emissions in Canada. (Data from [23])

The distribution of GHG emissions by sector and transportation-specific modes is shown in Fig. 2.7. With the considerable role of passenger car fuel combustion in emission levels, commuter transit—which effectively addresses traffic congestion and reduces pressures on infrastructure—is still reliant on the use of fossil fuels, and this results in GHG emissions. However, when placed in context with other forms of transportation, rail transit represents only a small percentage of the total GHG emissions in the Canadian landscape, making it a worthwhile endeavor to consider viable alternatives that are environmentally benign and/or neutral.

Although the rail sector is not a significant contributor in terms of total transportation sector GHG emissions, the locomotive fleet is fueled almost entirely by diesel fuel. Between 2009 and 2010, diesel consumption by railway operations increased

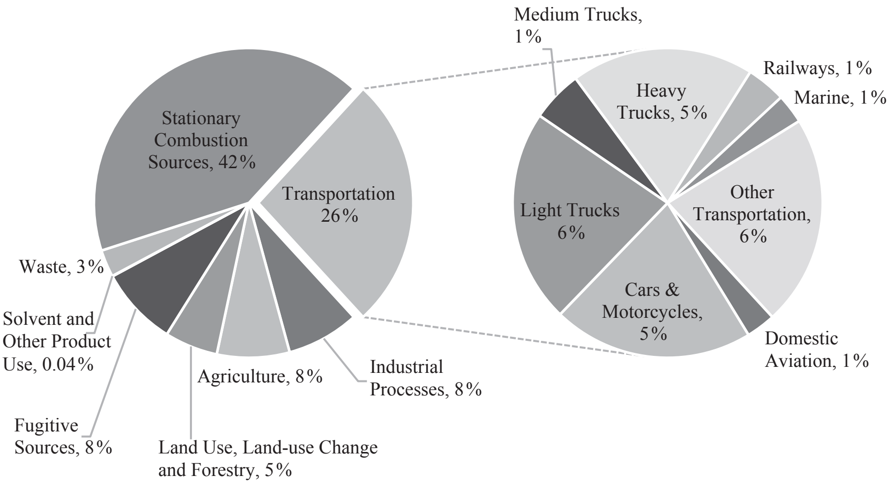

Fig. 2.7 GHG distribution by sector and mode of transportation, 2012. (Data from [24])

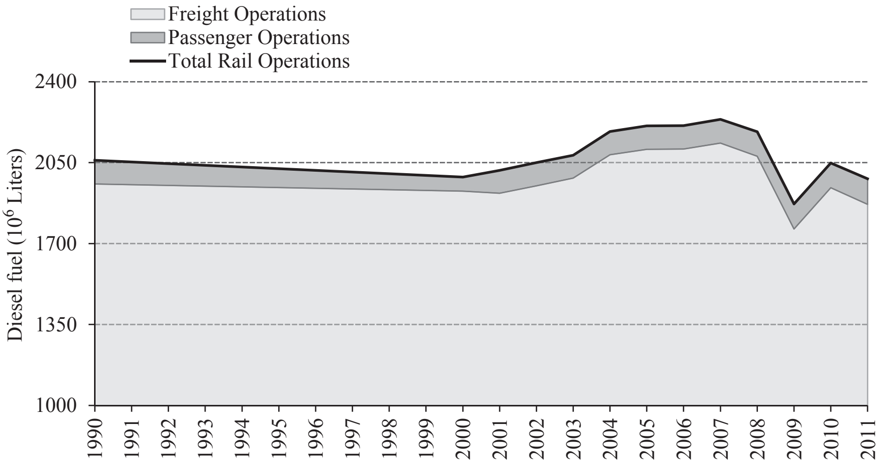

Fig. 2.8 Diesel fuel consumption by rail operation. (Data from [20])

significantly, from 1.87 billion litres of fuel to over 2 billion, due to increased freight operations (Fig. 2.8).

The emission of atmospheric pollutants leads to other harmful effects on the environment besides the global warming. These are illustrated in Fig. 2.9. There may be pollutant emissions, accidents, hazards, ecosystem degradation through air and water pollution, animal poisoning, greenhouse gas emission, carbon monoxide leakages, stratospheric ozone depletion, emission of hydrocarbon, CO, SO_2, NO_x, volatile organic compounds (VOCs), particulate matter (PM)(), and other aerosols. In average, the CO emissions are of 1.6 g/kWh, hydrocarbons of 0.81 g/kWh, NO_x of 9.5 g/kWh, PM of 0.22 g/kWh [17].

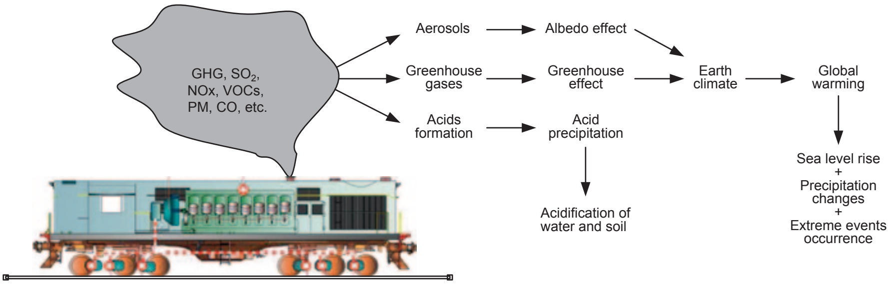

Fig. 2.9 Environmental pollution and effects from diesel combustion

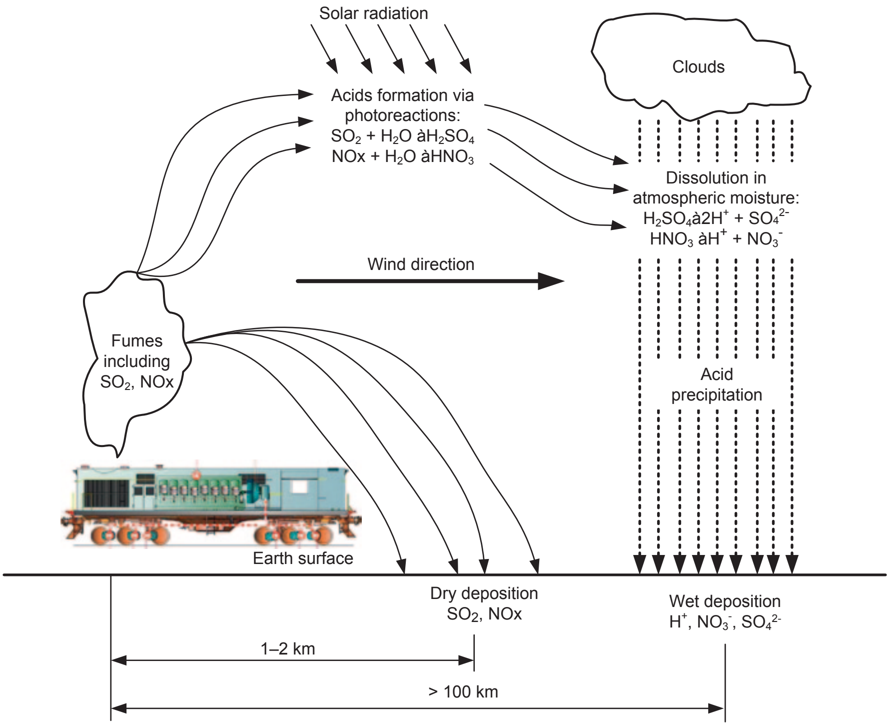

Fig. 2.10 Mechanism of rail transportation-related acid precipitation

A detail of acid formation in the atmosphere and acid deposition on land and sea is illustrated in Fig. 2.10. Acid precursors produced mainly from the combustion of fossil fuels, especially coal and oil, and the smelting of non-ferrous ores can be transported long distances through the atmosphere (by winds and currents) and deposited on ecosystems.

The majority of SO_2 and NO_x emissions come from fossil fuel combustion sources. Dry deposition of SO_2 and NO_x creates opportunity for acid formation at soil level or in the sea. Direct deposition occurs at places 1–2 km distant from the emission source. Acid precursors that travel to high levels of the atmosphere involve in

Table 2.2 Rail industry green house gas (GHG) emission intensities and Memorandum of Understanding (MOU) targets. (Source: [20])

Rail operation	Units[a]	2006	2007	2008	2009	2010	2011	%–Red.[b]	2015 Target
Class I Freight	kg/10^3-RTK	17.40	17.32	17.61	16.94	16.43	15.24	6 %	15.44
Regional and short lines	kg/10^3-RTK	14.77	15.22	15.80	14.20	15.21	14.88	3 %	14.75
Intercity passenger	kg/PAX-km	0.13	0.13	0.12	0.13	0.12	0.12	6 %	0.11
Commuter rail	kg/PAX	1.70	1.71	1.74	1.95	2.06	2.19	NA	1.46

[a] Units are expressed in terms of kg-CO_{2eq} per productivity unit; *RTK* Revenue ton kilometer, *PAX* passenger

[b] % Reduction from 2010 levels

the photo-induced reactions with water vapors and form acids such as sulfuric acid and nitric acid. These acids travel far from the source point of pollution and are dissociated in the atmospheric moisture. The dissociated acids fall on earth surface with precipitations.

Acidification and other type of pollutions caused by railway transportation may affect the quality of water including groundwater, because of its role in the supply of drinking and irrigation water. Economic priorities often cause the land, in particular, suitable for sustaining agriculture, housing, or natural ecosystems to be lost. Atmospheric pollution poses special health and environment threats, and is mainly generated by the chemicals and metal industries. The environmental impact of atmospheric pollution can be observed at the level of ecosystems, food, coastal regions, industry, settlements, and overall health.

To mitigate the effects of diesel combustion, emission reduction targets are set by the Railway Association of Canada (RAC) and Canadian government for all rail operations, imposing increasingly stringent GHG and criteria air contaminants (CAC) emission limits over time. Current limits, listed in Tables 2.2 and 2.3, are in line with those established by the US Environmental Protection Agency (US EPA), and are given in terms of emission intensity standards using a tiered approach based on the year of manufacture and specific mode of operation of a locomotive.

Table 2.3 Environmental Protection Agency (EPA) locomotive criteria air contaminants (CAC) exhaust emission standards (g/bhp·hr) (Source: [25]).

Duty-cycle	Tier	Year	HC	NO_x	PM	CO
Line-haul	Tier 0	1973–1992	1.00	9.50	0.22	5.00
	Tier 1	1993–2004	0.55	7.40	0.22	2.20
	Tier 2	2005–2011	0.30	5.50	0.10	1.50
	Tier 3	2012–2014	0.30	5.50	0.10	1.50
	Tier 4	2015+	0.14	1.30	0.03	1.50
Switch	Tier 0	1973–2001	2.10	11.8	0.26	8.00
	Tier 1	2002–2004	1.20	11.0	0.26	2.50
	Tier 2	2005–2010	0.60	8.10	0.13	2.40
	Tier 3	2011–2014	0.60	5.00	0.10	2.40
	Tier 4	2015+	0.14	1.30	0.03	2.40

2.5 Potential Solutions for Clean Rail Development

Constant research and development activity is observed in recent years toward determining the rail transport technology, which is more efficient and more attractive from economic and environmental point of view. At the same time, there is a general policy tendency to relate the railway transport to secure energy sources with less dependence on imports and fluctuating prices.

The improvement of the current diesel-electric locomotive is desired by governments, companies and public because with the current diesel-electric technology, the fuel price tends to escalate (~30% increase in 2011) and the air pollution is significant. Potential technological options/solution for clean rail that will reduce the environmental impact and cost and increase efficiency and effectiveness must be investigated. These may lead to more sustainable rail transportation systems in the rail sector. In the recent decade, various fuels and fuel combinations were proposed for clean rail locomotives, such as hydrogen, CNG, LNG-Diesel, LNG-LPG, LNG-H_2, etc.

Among other options, the investigation of alternative approaches for smart energy management of liquefied natural gas (LNG) locomotives. Novel schemes for efficiency improvement and air pollution reduction are disclosed and assessed, such as partial fuel reformation with heat recovery from exhaust gases. Novel interfaces between tender LNG railcars and locomotives and alternative ways to reduce the energy losses due to methane venting, which is normally required for maintaining LNG storage for a long time, should be developed.

Recent technological advances led to successful demonstration of LNG locomotive propulsion system by Canadian National with a 480 km test-ride in Alberta. With this demonstration, the LNG in rail transport becomes a game-changer because fuel cost is cut to half when compared to diesel-electric, while reducing the air pollution by approximately 25% and increasing the driving range up to two times. However, adopting the LNG locomotives becomes extremely challenging due to the following drawbacks:

- A unitary LNG powering system must be developed and should assure interoperability and interchangeability of line-haul locomotives among major freight railroads in North America.
- A smart energy management system must be developed to perform multiple functions in a more efficient and effective manner and maximize the locomotive and railcar driving ranges.
- A method for handling cryogenic liquid in large volume (> 100,000 L) must be selected for avoidance of boil-off methane venting and consequent LNG weathering as a well as for engine proper fuelling.

The retrofit of the diesel-based line-haul locomotives to LNG is a proven concept after a successful demonstration done by Canadian National Railway Company in 2012 when two-paired locomotives where connected to a LNG tender and rode 480 km in Alberta on 90% natural gas and 10% diesel as ignition promoter. There is an important drive toward the use of LNG in railway transport (especially for freight) which is justified by economical, ecological, and societal factors. The LNG price is lower than diesel with the potential of making two times cheaper rides, the GHG emission from LNG can be reduced with respect to diesel provided that innovative energy management technologies are applied. An improved air quality can be definitely obtained when LNG rails are adopted at continental scale, and this definitely brings an important societal benefit.

Since no LNG infrastructure is in place for railroads, the range of line-haul locomotives for freight transport should be extended beyond 4000 km, which will minimize the investment in liquefaction stations, or otherwise the powering system must be able to operate in diesel-only mode. In order to travel such longer distances (double those of systems in place), the LNG locomotive must run more efficiently than the diesel-electric system.

There are two established concepts to convert the current two-stroke diesel engines for locomotives to LNG. In a low-pressure approach established in the 1990s by the American company Energy Conversion Inc., natural gas vapors are extracted from the LNG tender car and then heated and injected into the two-stroke engine through a special low-pressure injector that opens immediately after the intake port is closed. The natural gas fuel is compressed together with air, and then a small pilot injection of diesel fuel is given at the top dead end to ignite. This system has major benefits because it reduces NO_x emissions; since injecting less diesel lowers the combustion temperature, it eliminates the need of boil-off methane venting because cryogenic vapor are drawn from the tank for fuelling. Although this system is safe and allows for dual operation (diesel-only or LNG-diesel) , there is a technical difficulty as the required injection pressure should be higher than 7 bar (absolute). However, during the operation, the pressure in the cistern can reduce or fluctuate, and suddenly the engine remains without fuel.

Westport Inc. came up with a fuelling solution that allows natural gas supply at controlled pressure from the cryogenic tank [26]. They use a positive displacement pump that will displace a two-phase mixture. The vapor/liquid fraction at pump intake can be adjusted automatically in function of the needs. Although Westport applied this solution for high-pressure injection systems (200 atm), then it can definitely work for low-pressure injection systems as well. The fuelling system promoted by Westport and known as high-pressure direct injection (HDPI) injects natural gas in the late compression stroke. An integrated system is proposed by Westport that includes a fumigated low-power engine supplied with the boiled-off LNG, which turns a cryogenic pump to pressurize the liquid fuel up to 200 atm for injection. Nevertheless, the major disadvantage of the HDPI engine is that it is not designed for diesel-only operation, and, therefore, this system is closely related to the LNG infrastructure development.

It is clear that the requirements for adopting a unified LNG locomotive system pose severe challenges to research and development. In a perfect engine design, one must have an excellent balance between cryogenic liquid handling, fuel preheating and injection, controlling combustion parameters according to the load, heat recovery, and emission control. Although the internal combustion engine for LNG locomotive is at the verge of commercialization based on HDPI technology, other alternative systems should be considered. Solid oxide fuel cell (SOFC) appears very attractive for locomotives. The great advantage of the SOFC is that they can be fuelled directly with natural gas as there is no need of diesel, and in addition, the electric generator can be eliminated. However, the technical challenge is to design a compact fuel reforming unit that should fit the size of a typical locomotive.

System integration and energy management appears to be the secure pathway that eventually leads to the establishment of a LNG locomotive system that is widely adoptable. Natural gas can be fed directly to solid oxide fuel cell, and advanced heat and work recovery can be obtained by cascading the SOFC with gas turbines. Multiple options for energy management for locomotive should be known and assessed as a prerequisite step before the eventual adoption of the most successful ones.

Another development option for locomotives is the diesel/methanol co-fueling as a better fueling system with improved efficiency, improved economy, and reduced environmental impact. The system is applicable both to the rail transport locomotives and to the rail yard switcher locomotives. Some modifications to the locomotive balance of plant and placing two fuel tanks (diesel and methanol) instead of one are required.

The use of methanol as a fuel for general purpose compression ignition engine has been studied in the past and its feasibility is confirmed as shown in the review paper from Ref. [27]. However, the use of methanol to enhance diesel fuels for locomotives has been scarcely studied in the past. In Ref. [28], methanol has been even cited as an alternative railroad fuel that reduces railroad costs. Direct injection of methanol fuel is reported in Ref. [29] for a two-stroke locomotive engine converted to methanol as a primary fuel and pilot injection of diesel fuel as ignition. The scientific results of [29] show that methanol with diesel pilot produces similar energy efficiency as diesel locomotives.

When methanol-diesel is used to fuel locomotives the reduction of atmospheric pollutants such as greenhouse gases, NO_x, SO_2, particulate matter (PM), and volatile organic compounds (VOCs) is drastically reduced because less carbon dioxide is found in the flue gases and the combustion temperature is generally lower, not permitting the NO_x formation. Furthermore, methanol as a synthetic fuel is cleaner, henceforth SO_2, PM, and VOCs emissions will be reduced.

Methanol has been proposed as an alternative to current petrochemical fuel-based economy by the Nobel laureate George Olah. Methanol can be produced either from petroleum or from renewable energy sources, which is a major advantage for sustainable development. The "ingredients" to produce methanol with renewable energy are water and carbon dioxide, which can be recovered from stack gas emissions. Alternatively, methanol can be produced from biomass. Therefore, renewable methanol is a carbon-free fuel.

Hydrogen has been called "the energy carrier of the future." However, major challenges exist in hydrogen storage and the development of a fuelling infrastructure is extremely costly. For example, hydrogen presents an explosion danger as it is highly flammable; requires compressed storage with explosion risk and associated compression costs, and also has low-energy density.

Ammonia-based locomotives for passenger trains in the existing rail infrastructure have been proposed recently, where ammonia can be used either as a hydrogen source or as a fuel. Ammonia confers better compactness, longer raids, better cost effectiveness, and increased safety than the onboard fuel tank of hydrogen locomotives. In addition, the infrastructure for ammonia fuelling of locomotives is cheaper and safer than a hydrogen fuelling infrastructure. Ammonia is a safe, non-flammable, highly efficient, carbon-free, environment-friendly alternative fuel that is cheaper than diesel, and can be well used for locomotive propulsion. Ammonia can be synthesized using renewable sources starting from hydrogen extracted from water and nitrogen extracted from air. Expelled gases from the system are only steam and nitrogen, and there are no carbon emissions, unlike other hydrocarbon fuels, including diesel. Ammonia acts as a nitrogen oxide (NO_x) reduction agent, thus there will be none or very reduced NO_x emissions.

The ultra-low sulphur number 2 diesel used for rail transportation shows an increased price trend with a rise of 28.2 % in 2011. Ammonia, as a fuel, costs US$0.55 per liter off the grid [30], and even cheaper if powered by wind farm. This represents at least 32 % cost is saved if diesel was replaced with ammonia, or US$450 million based on the average annual cost of US$1.4 billion. Ammonia can be used in any locomotive internal combustion engine that works with hydrogen; hydrogen-ammonia mixture; direct ammonia fuel cell; or hydrogen-fuelled fuel cells. There is a global demand to reduce carbon emissions and greenhouse gases, and as such alternative fuels that reduce emissions while also diminishing the operating costs of the railway system are highly desirable.

An ammonia-based locomotive fuelled system would include an ammonia decomposition, and the separation unit thermo-catalytically cracks (partially or totally depending on the case) ammonia to hydrogen and nitrogen using low-energy recovered from combustion gases. The system can be used either to generate pure hydrogen to fuel the fuel cells for locomotives, or it can generate a tuned ammonia-hydrogen mixture with combustion properties similar to that of conventional fuels, which can be supplied to an internal combustion engine. The expelled gases are only steam and nitrogen, both are environment-friendly. Furthermore, the system can take advantage of the unique properties of ammonia to be a refrigerant, fuel, and NO_x reducing agent. Thus, the system can also generate cooling for air conditioning or for the engine temperature control, and as well it can self-reduce its NO_x emissions such that the tailpipe expels only nitrogen-enriched air and steam.

The ammonia tank will be cheaper, lighter, less voluminous, and safer than the current hydrogen tanks since it confers 97 % reduction in storage pressure. Ammonia has a high energy density; it has an existing distribution network with over 100 million tons being distributed annually, and ammonia rail cisterns are very well developed. Ammonia is not considered flammable when properly transported, and is considered safer than various fuels including conventional fuels, compressed natural gas, methanol, propane. Its gas-phase density is smaller than that of air, and it dissipates rapidly if it escapes into the atmosphere. It is also self-alarming, as any leakage can be detected by nose in concentrations as low as 5 ppm.

2.6 Illustrative Example: Commuter Rail Transit in the Greater Toronto Area

As one of the most highly populated cities in North America, Toronto and the surrounding the Greater Toronto Area (GTA) has the most extensive diesel locomotive commuter rail network in Canada [26]. The GO transit, a division of Metrolinx, provides regional public transit service for the GTA and Hamilton Area with passenger trains and buses across 11,000 km^2 [31]. The GO rail system is one of Canada's largest commuter rail networks, handling for 185,000 passengers on weekdays, operating 47 locomotives.

The rail network details are shown in Fig. 2.11. At full capacity, one locomotive is able to carry the same number of passengers as 1670 cars based on an average of 1.15 passengers per vehicle during rush hour [32], indicating the potential for commuter rail to reduce urban traffic congestion. While the rail transit systems like the GO rail commuter fleet provide attractive alternatives to personal vehicles, this system, and similar systems across Canada, continues to rely on fossil fuels and GHG-producing technology to function. As part of a continuous effort to reduce GHG's from locomotive exhaust in the GTA, Metrolinx is in the process of converting Tier-2 locomotives to meet Tier-4 limits by upgrading emission control technologies, with in-service testing of ten locomotives estimated to begin in 2015 [20].

The GO rail commuter fleet includes 65 Tier-2 emission compliant MP40PH-3C diesel-electric locomotives, capable of pulling/pushing 12 bi-level passenger coaches. The transit system operating details are given in Table 2.4. Ammonia fueling is considered for use in GO rail operations, and the potential of the ammonia fueling is addressed for overall fuel cost and environmental performance.

The relationship between levels of GHG emissions and transportation emissions is well-established in the Canadian example, with contributions from the transportation sector representing the largest portion of GHG emissions by economic sector in Canada, at ~25 % of the national total in 2012. With road vehicles, such as heavy duty freight trucks, light duty trucks, and light (passenger) vehicles, contributing to the majority of GHG emissions within the transportation sector—primarily due to the combustion of fossil fuels,practical solutions for the integration of more environmentally benign options for passenger transit are an important and necessary area for exploration. However, solutions that aim to address the GHG-producing technology utilized in the operation of passenger vehicles, but which do not address the prevailing social, cultural, and economic factors that contribute to the dominance of fossil fuels as the primary choice for personal transportation, do little to reduce the environmental impact of the high-density on-road traffic that characterizes many of Canada's urban centers.

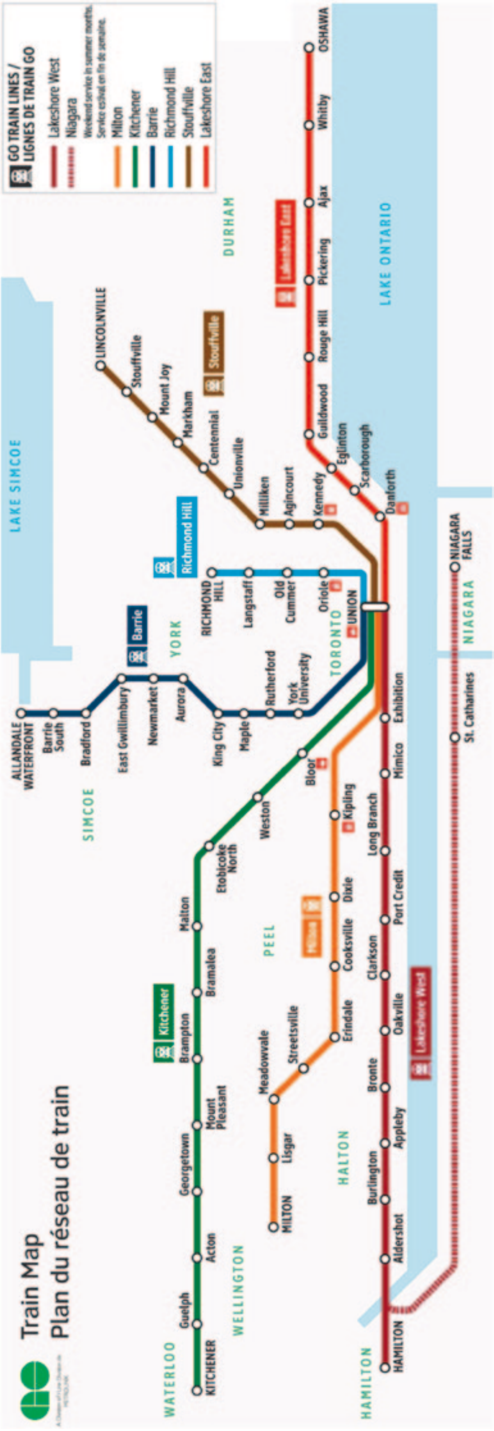

Fig. 2.11 GO train map in greater Toronto area [32]

Table 2.4 The GO rail transit system details. (Source: [32])

Passengers (weekday)	185,000
Number of lines	7
Stations	63
Route length	450 km
Weekday train trips	203
Weekday train-sets in use	47
Locomotives (MP40PH-3C, Tier 2)	65
Bi-level passenger coaches	563 (162 seats)
Fuel capacity	8410 L

2.7 Closing Remarks

Rail transportation presents a practical, efficient, and realistic alternative to passenger vehicles and freight transport. In many cases, an existing, operational system is utilized in urban and suburban centers worldwide. In the best case scenario, commuter and intercity trains provide a comfortable, predictable, and affordable alternative to cars or other light vehicles, and on a broader scale, move large numbers of passengers quickly and efficiently with a considerably smaller environmental impact. This is just at $\sim 1\,\%$ of the total GHG emissions in 2012 in the Canadian illustrative example given above.

Furthermore, as an attractive option for business and personal travel alike, commuter trains have the potential to reduce the number of passenger vehicles utilized for transportation, the related wear and tear on roads, and other infrastructures required for car travel, and traffic congestion and density, particularly in densely populated urban centers.

Chapter 3
Locomotive Prime Movers

3.1 Introduction

Railway transport development is tightly bonded to the development of the locomotive movers. The invention of the reciprocating steam engine in the eighteenth century was the key element that led to the apparition of rail locomotive and railway transport. The early development of boiler technology allowed for the creation of the non-condensing steam engine technology which by late 1700s and early 1800s was installed on railway locomotive. This well-known prime mover required a large-size pressurized steam generator fired with coal stored in a tender wagon. The railway lines expanded because the prime mover facilitated the transport of construction materials and personal creating thus the infrastructure.

After 150 years of domination, the steam locomotive was replaced with a more competitive prime mover, the diesel engine. After 1950s, the technological development allowed for a fast expansion of diesel locomotive and a gradual disappearing of the steam locomotive so that, today, the majority of railway locomotives are powered by diesel engines. The diesel-electric locomotives are proven to be more effective than the diesel-mechanical and become the most spread technology used today for railway transport.

The prime mover of the diesel-electric locomotive is still a diesel engine, which is integrated with a power generator and a set of electric motors for propulsion. The economic factors show that in most of the cases, a diesel-electric locomotive outperforms the diesel-only because less complicated mechanical systems are required by the first. Furthermore, the diesel-electric system allows for full hybridization such that regenerative braking can be applied and energy recovered in batteries, which leads to important savings.

The electric-only locomotive represents the only competitor of the diesel-electric one for current railroads. The electric-only locomotive appears to be the most efficient prime mover. The locomotive is connected to the power line and uses a DC or AC

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motor as a prime mover. The electromechanical power conversion is very efficient. No flue gas emissions are expelled in the atmosphere, the only pollution source being due to the power generation process of the local grid. The only downside of electric locomotive is related to the construction effort, measured in terms of both financing and indirect environmental impact. The installation and maintenance of the electric lines are expensive, whereas this price component is nonexistent for non-electrified railways. In this way only, a minority of railroads in the world are electrified.

In this chapter, the conventional locomotive prime movers are reviewed. A historical perspective on the evolution of prime movers from the beginning of their development until the ones in use today is given. The prime movers from all segments of railway operations including passenger and freight transport and car switching operations are discussed. The technical features of the relevant locomotives are also presented with some examples.

3.2 Historical Perspective

As it is generally known, the earliest system of railways was developed in England by George Stephenson in about 1830 initially in the form of a public passenger transport system traveling from Liverpool to Manchester. This revolutionary development was in fact possible due to another technical revolution, namely the invention of steam engine prime mover and its technological development, during the eighteenth century.

Stephenson eventually succeeded in creating an effective locomotive and railway system. The locomotive was equipped with a non-condensing steam engine. This prime mover produced high-pressure saturated steam which was then expanded into a reciprocating steam engine mechanism and released into the atmosphere. There are several key technical features of this prime mover which are worth attention, such as the development of a high-pressure steam generator, the reciprocating piston, and the crankshaft mechanism.

The precursor of the reciprocating steam engine was invented by Thomas Savery by the very end of 1700s. The Savery engine was in fact a no-piston mechanism capable of lifting water by using the force of steam. The pressure vessel technology was not known at that time; therefore, the machine of Savery could not relate to the pressure of steam, but rather to the vacuum creation with the help of steam which is condensed in a sealed vessel. The system developed by Savery is schematically illustrated as shown in Fig. 3.1.

If we look at this system, we see that it consists of two sealed vessels and three valves. As it can be easily understood from the figure, steam is produced in a first vessel heated by fire from the bottom. The vessel is filled with water which boils to generate steam at slight overpressure. The second sealed vessel works intermittently in vacuum and slight overpressure; this vessel is denoted as the working cylinder. When water in this vessel is at high level, the valve V_1 is shut off and valves V_2 and V_3 opened. Steam is admitted into the vessel, and as steam is continuously gener-

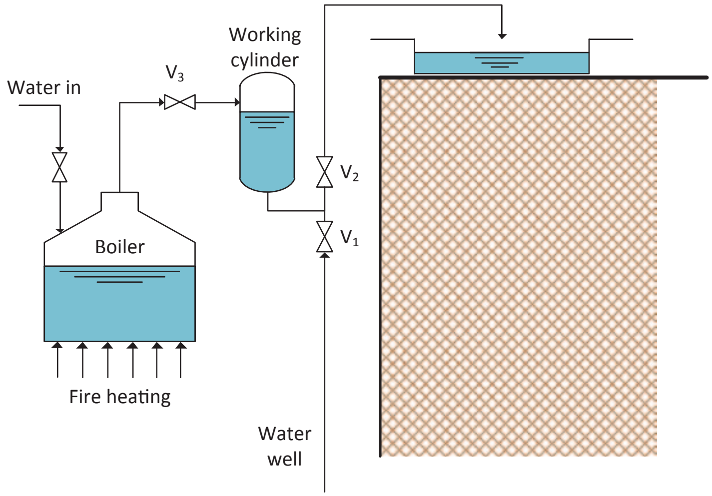


Fig. 3.1 The precursory of the reciprocating steam engine—the Savery water pump

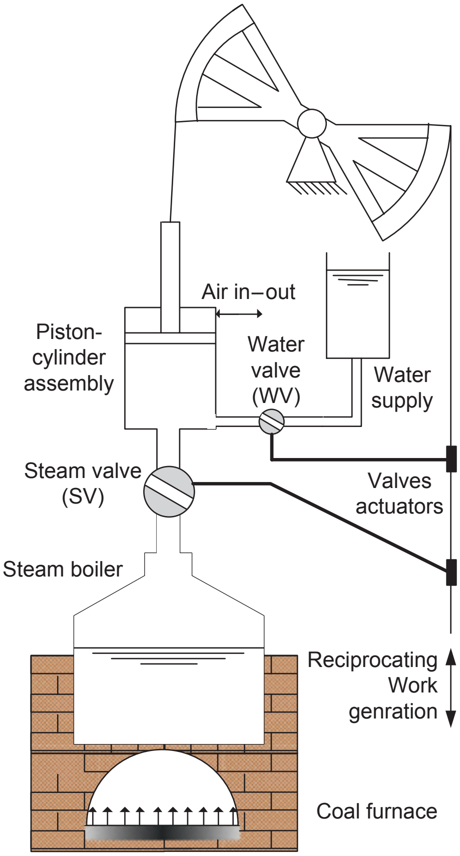
ated, it impinges water down, tending to occupy more space. Therefore, water exits from the vessel and is discharged at the high level. For the next phase, the steam admission valve V_3 and water release valve V_2 are shut off and the working vessel isolated. Then, the working vessel is cooled either by air in natural convection or by showering some cooled water over it. Once the vessel is cooled, steam condenses in it, and since the vessel is sealed, a vacuum is created. Once the vacuum is sufficiently deep, the water admission valve V_1 is opened so that new water is pulled up from the well until the vessel is filled.

The Savery steam pump proved beneficial at that time for mining operations which required large amounts of water to be removed from the pit. The Savery engine—also known as Savery water pump—started to be used extensively at the very beginning of 1700s.The main limitation of this water pump is its suction type of operation. Technically, this pump cannot be used to displace water for more than approximately 9 m height. Another aspect is due to the high energy losses in the working vessel caused by the intermittent operation as a condenser and as a working cylinder.

Three inventions that occurred by the end of 1700s and attributed to Denis Papin (an assistant of Boyle) were proven crucial for the further improvement of the Savery steam engine. These are the pressure cooker, the steam pressure valve, and the pneumatic cylinder–piston mechanism. The pressure cooker and steam pressure creation contribute definitely to the development of pressurized steam generators. The pneumatic cylinder–piston mechanism has been integrated by Thomas Newcomen in England into the Savery steam engine. The application of piston–cylinder mechanism has been the key improvement to the Savery heat engine.

Figure 3.2 shows the operating principle of the Newcomen reciprocating engine. The engine uses vacuum rather than pressure to generate a reciprocating move-

Fig. 3.2 Reciprocating engine of Thomas Newcomen



ment. Similarly, as for the Savery system, a furnace is used to generate steam in a large vessel at slight overpressure. Steam is aspired into a cylinder when the piston displaces upward. When the top dead end is reached, the water valve (WV) opens, allowing the cold water to enter the cylinder. Once it enters, a cooling effect is produced by direct contact with steam, and, therefore, steam starts to condense and pulls the piston down. While moving downward, the two valves controlling the piston–cylinder mechanism are shut off. Under the force of the vacuum, the power stroke of the engine is developed, which eventually ends when the piston reaches the lowest position. At this time, the steam valve is automatically opened by the mechanism allowing for steam to enter into the cylinder and break the vacuum. The balance of water is maintained constant inside the system.

James Watt made, by 1760s, a crucial improvement to the Newcomen concept, namely the addition of a separate condenser. The fuel economy of condensing Watt engine has become superior to that of Newcomen although the engine still operates at slightly atmospheric pressure. The improvement in efficiency relates to the fact that the cylinder and piston mechanism is maintained hot, while the condensation of

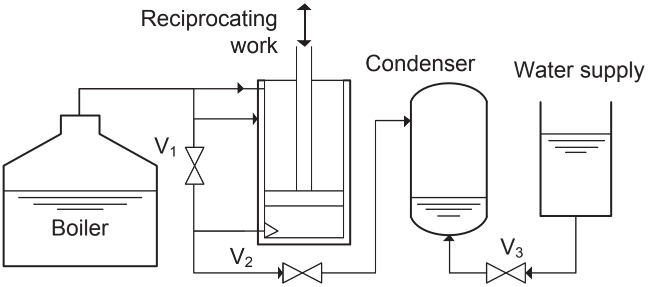


Fig. 3.3 Operating principle of the reciprocating condensing steam engine of Watt

steam and thus the vacuum is conducted in a separate vessel. In addition, the design limited the air penetration into the piston by injection of steam continuously at the highest pressure side of the piston.

Figure 3.3 shows the principle of the reciprocating condensing steam engine developed by Watt. The slightly pressurized steam is admitted into the cylinder through valve V_1 when V_2 and V_3 are closed. The forces at the two sides of the piston being slightly unbalanced push the piston upward. Once being at the top end, V_1 is shut off and V_2 and V_3 are closed. Steam then expands and moves into the condenser which is kept at vacuum. Because the condenser is at vacuum, cold water enters at the bottom of the condenser passing through valve V_3. In contact with cold water, steam condenses rapidly and the vacuum is maintained. Therefore, the piston is pulled down under high force, this being the motor stroke of the engine. After a while, the condenser fills with water but this can be pushed out by blowing steam from the boiler whatever the case is. Therefore, air penetrations are avoided and no special pump is required. If the boiler vessel runs out of water, the steam pressure valve is opened to release pressure and more water is admitted again, without the need of a pump.

James Watt together with his collaborator William Murdoch made a subsequent major improvement to the steam engine by applying the sun and planet gear (a precursor of the slider-crank mechanism) to convert the reciprocating movement of the steam engine into a rotational movement. Further, Watt invented the double acting steam piston, the centrifugal governor, and pressure gauge and integrated them into the steam engine.

Some attempts existed in the second half of the eighteenth century to install the steam engine on a carriage and develop a road locomotive. However, a massive and heavy engine such as that of Watt has been difficult to install on a vehicle. William Murdoch attempted and succeeded to develop prototype of higher pressure steam generators and develop the non-condensing steam engine which has been lighter so that he installed it on a road vehicle and demonstrated the road steam locomotive. Richard Trevithick further developed the high-pressure steam engine and achieved to install it for the first time on a rail locomotive for mining operations. The non-condensing high-pressure steam engine for rail locomotive became a commercial success for industrial application during the very first years of nineteenth century.

George Stephenson constructed, by 1810, a mining locomotive able to haul couple of tons of coal; he also contributed to the development and implementation of iron rails to construct railways and introduced the idea of using multiple wheels for locomotives such that the weight is distributed in a better way. The railway gauge of 1435 mm used at that time by Stephenson has been adopted as standard for railway construction worldwide.

By 1825, a longer railway was established under the supervision of George Stephenson carrying coal between mines near London. This railway is known as Stockton and Darlington railway. The locomotives developed for this railway were able to haul nearly 100 tons of coal in wagons at a speed of over 30 km/h. On this railway, the first-ever passenger wagon was tested and used. The application of fire tube steam generator has been essential for the improvement of heat transfer surface and efficiency of the locomotive system.

Figure 3.4 shows the portraits of the pioneers of railway transport covering the period from the early steam engine prototype of Savery to the first-ever Liverpool–

George Stephenson
1781–1848

Thomas Savery
1650–1715

Thomas Newcomen
1664–1729

James Watt
1736–1819

William Murdoch
1754–1839

Richard Threvithick
1771–1833

Fig. 3.4 Prominent pioneers of rail transport and locomotive systems

Manchester public railway opened by Stephenson. After 150 years of marked domination, steam locomotives became obsolete and are completely replaced, nowadays, by diesel-electric locomotives. In some limited regions, electric railways are constructed which allow for the use of electric-only locomotive. Depending on the specific application, the locomotive design and its engine capacity vary: Switching locomotive has small capacity engines, whereas hauling locomotive is designed generally for high power output at MW level.

3.3 Classification of Prime Movers

The mother of public transportation is known as rail transport for passengers and goods. When it was discovered and implemented, it was the primary way of transporting passengers and goods. The prime movers for locomotives are basically classified into five categories as shown in Fig. 3.5 which can also be read as the evolution of locomotives. The alternative locomotive prime mover includes a variety of types presently under research and development such as hydrogen fuel cell locomotive, compressed and liquefied natural gas locomotives, ammonia locomotive systems, battery-only locomotive, and others.

It is known that steam engines were the driving force behind industrial revolution and powered machineries in mills, factories, plants, etc. The ultimate target was to apply the pressurized steam ships, locomotives, and several other types of vehicles. So, the history of rail sector began with steam locomotives with the aim of transporting people and goods faster and safer from one location to another in much greater quantities and much shorter time. This helped developing cities and their economies. Later, diesel engines became much less expensive, much more reliable, much quieter, and much more effective to carry larger amounts of goods and apparently caused steam locomotives to disappear.

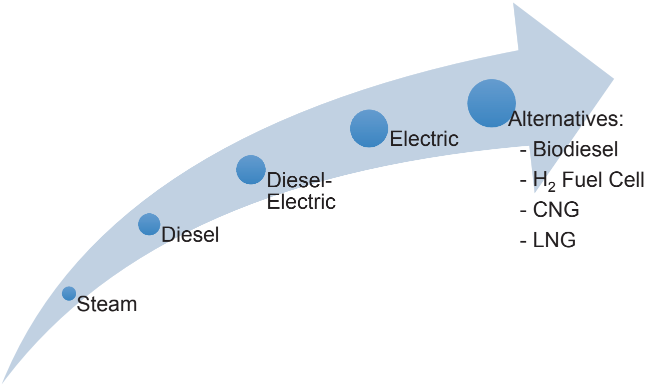


Fig. 3.5 Evolution of locomotive prime movers

These diesel locomotives were primary option of rail transport in the world from North America to Europe and from Europe to Far East and continued their predominant role up until after the end of Second World War. Hereafter, diesel electric was used together to have advantage of electric motors in a combined manner to make the rail transport more efficient, cost-effective, and environmentally benign.

One should note that many hybrid locomotives at present use dual engines which can help harness the power of electrical grid in urban areas and use diesel engine in more harsh terrains outside the cities. Of course, electric locomotives have been an ultimate option in rail sector, due to advances in electrical grid infrastructure and electric motors manufacture enabled trains to adopt electrical power as one of the most reliable and effective sources of propulsion. Today, electrical locomotives are employed everywhere, from city transit trains, subways, trams, to high-speed rapid transit trains.

3.4 Steam Locomotives

Although there were several pioneers of steam locomotive, as reviewed above, George Stephenson can rightfully be called the “father” of this technology. Being both a mechanical and civil engineer, George Stephenson succeeded to contribute essentially not only to the locomotive development itself but also to the technology of railway construction. Probably, the major contribution by George Stephenson and his son Robert was the incorporation of the firebox within the steam generator and the flue gas pathway designed at the full diameter of the cylindrical boiler. This kind of design proved so successful that it became the standard arrangement for the conventional steam locomotive as shown in Fig. 3.6.

The pressure in the boiler has been kept at few atmospheres. The firebox is surrounded by a water jacket as shown in the figure. The hot flue gas flows through

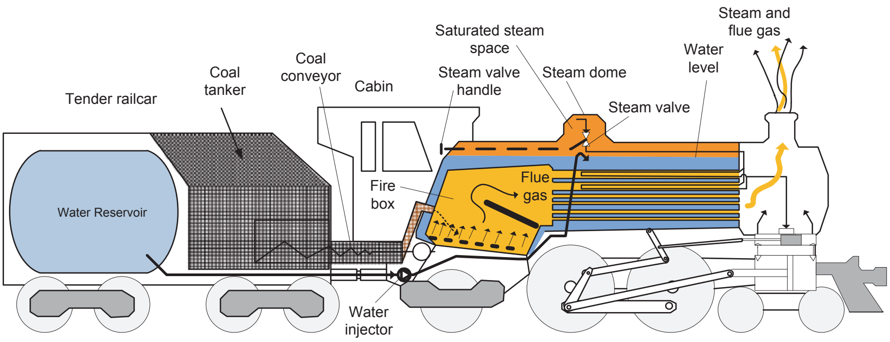


Fig. 3.6 Conventional steam locomotive prime mover

Table 3.1 Stephenson's locomotive prime movers. (Source: [33])

Name	Year	Configuration[a]	Axle load	Weight
Northumbrian	1830	0-2-2	2.9 t	11.6
Planet	1830	2-2-0	2.18 t	4.32
Patentee	1835	2-2-2	3.8	11.4
Adler	1835	2-2-2	3.8	11.4
Le Belge	1835	2-2-2	3.85	11.56
De Arend	1839	2-2-2	3.9	11.7

[a] Configuration based on Whyte notation: number of leading wheels-driving wheels-trailing wheels

pipes immersed in water and reach into the other side after transferring sufficient amount of heat to the water which boils in a pool boiling process. The volume of water is maintained constant with the help of an injection pump. A valve actuated by the operator allows for the control of the saturated steam extraction in accordance with the need of power.

The saturated steam is superheated by the hot flue gases and then provided to the piston–cylinder mechanism which is controlled by the timing valve. The low-pressure steam after expansion exits through the chimney together with the flue gases. The air intake at the firebox is from below the grate. The feed of coal must be correlated with the engine load. Some of the locomotives built by George Stephenson were known as the Rocket, Northumbrian, Phoenix, North Star, Planet, Patentee, Adler, and De Arend; their main characteristics are given in Table 3.1.

These first UK locomotive models were exported throughout the world. The first American-built locomotive has been Tom Thumb made by Baltimore, and Ohio Railroad followed in 1830 by the locomotive "The Best Fried of Charleston" built by the South Carolina Railroad. The infrastructure for the steam locomotive railway has been quickly developed and included among other items: the water towers to refill the locomotive tenders with water at special stops, fuelling places, and maintenance depot.

The steam locomotive operation was relatively expensive due to its need of frequent maintenance for the mechanical units and a large number of crew persons (two operators, the driver and fireman, and traveling support crew). In addition, steam locomotives could not be standardized, but rather their designs were adapted to the requirements of specific railways. Due to the high indirect costs (e.g., maintenance, infrastructure) and low efficiency, the steam locomotive could not compete with diesel and nowadays became obsolete. For instance, diesel locomotive brought on the scene the advantage of traction modularity; that is, it allows synchronizing multiple locomotives to pull a line-haul train. All diesel locomotives of a line-haul train are controlled by only one crew of two persons, fact that is practically impossible for steam locomotive. Moreover, for yard switching operation, a diesel locomotive can be operated by a single person.

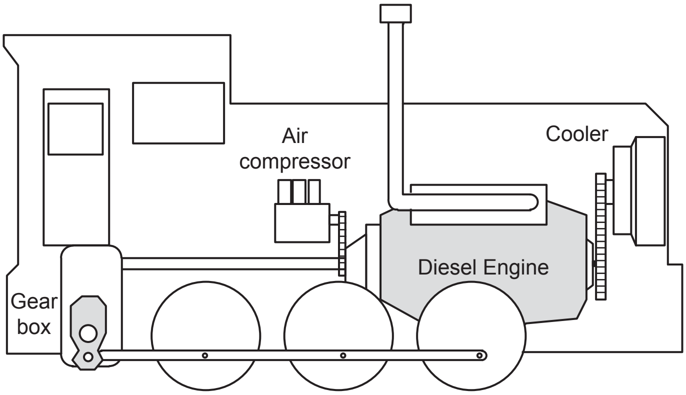


Fig. 3.7 Diesel locomotive prime mover

3.5 Diesel Locomotives

The diesel-only locomotive consists of a diesel engine that mechanically drives the wheels. The configuration is as shown in Fig. 3.7. The engine is either turbocharged or a compressor is used to provide the required air. A clutch system and a gear box are driven by the motor shaft. Parallel transmission with a crack system is typically used for draining the wheel. Many design variations exist, depending on the specific utilization of the locomotive. As of today, the diesel-mechanical locomotive is used for switching operation mostly. Their operational and investment costs were definitely cheaper than those of the former steam locomotives.

Diesel-mechanical locomotives were developed first for rail yard operation where they are proven very effective. They have the ability to switch fast between driving modes such as forward, backward, fast forward, slow forward, and idle, which is very convenient for car switching, trains compounding, maneuvers, etc. In addition, diesel locomotives require very short warming-up time and can immediately be started up to react with scattered tasks for rail yard operations. On the contrary, a steam locomotive cannot be maintained in idle mode for long periods of time. This is not economical since in idle mode, fuel is consumed. This is the reason why the number of the produced diesel switcher locomotives grew exponentially after the first diesel locomotive testing in Western Europe by 1920.

Relevant diesel-mechanical railcars development between 1920 and 1960 is briefly described here:

- In Hungary, Ganz factory produced a fleet of more than 100 of diesel railcars for local passenger transport from 1920 to1940.
- In Germany, the company Wismar constructed approximately 60 diesel railcars in the decade of 1930s.
- In France, Renault produced about 100 diesel railcars starting with 1933.
- In Italy, Fiat built diesel railcars starting with 1930, for a 20-year period.
- In Canada, Beardmore Company produced by 1930s passenger diesel railcars.

The propulsion power of the diesel-mechanical locomotive is limited to approximately 1.5 MW. This limitation is due to the mechanical transmission system which was difficult to be designed with a reasonable size for heavy trains requiring traction power of 3–4 MW or more, due to a high torque requirement. This was the reason why the diesel-electric locomotive was developed, as commented in the next section.

3.6 Diesel-Electric Locomotives

A diesel-electric locomotive functions as a power plant, generating its own electricity. It gets its power by using a diesel motor, which runs a generator which produces electricity to drive traction motors that turn axles and the wheels of the locomotive. When this is done, a high torque can be developed by the electric motors. The torque developed by the electric motors will be sufficient for propulsion of long/heavy trains from zero speed to high speed, accommodating traction powers of 4 MW or more. The electric motors are controlled by an inverter which can adjust the torque and rotation speed according to the actual traffic conditions.

The basic arrangement of a modern diesel-electric locomotive is shown in Fig. 3.8. During operation, shaft power produced by the diesel internal combustion engine (ICE) directly drives the engine governor, cooling water and oil pumps, radiator fans, and air compressor(s) of the locomotive, as well as electric generator(s) used to power the traction motors and various other cooling subsystems and locomotive controls.

An auxiliary generator charges a set of batteries, which supply power to the engine starter motor. In a diesel-electric locomotive, the diesel engine drives either an electrical AC generator/rectifier system or a DC generator which provide DC power to an inverter which can then drive the traction motors in a controlled manner. Therefore, there is no mechanical connection between the engine and the wheels.

The traction motors are generally AC electrical motors connected to four or six traction axles. The passenger and speed freight locomotives generally use four trac-

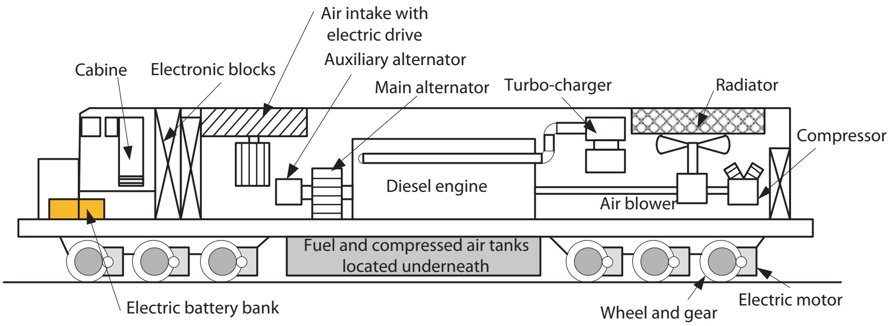


Fig. 3.8 Diesel-electric locomotive arrangement

tion axles, whereas the heavy low-speed freight trains use prime movers with six axles. The main alternator and the secondary alternator are connected to the diesel engine through elementary gear boxes installed on the main shaft. The diesel engine is turbocharged. The turbocharger will raise the pressure of the air at the intake manifold, and thus, the engine performance is improved. An aftercooler is installed to decrease the compressed air temperature before the intake into the cylinders.

Also, an engine radiator and an oil cooler are installed and driven mechanically by the engine shaft. The engine also drives an air compressor and hydraulic pump required for different actuation purposes. A head end power (HEP) engine (not shown in the figure)—typically a smaller diesel ICE—is used for cooling/heating systems and other "hotel power" operations within passenger occupied railcars. The HEP-ICE operates constantly, regardless of the locomotive engine speed.

Originally, on diesel-electric locomotives, the traction motors and generator were DC machines. However, once the high power electronics became commercially available, the DC generator has been replaced with a brushless AS alternator characterized by a reduced maintenance due to the elimination of the brush commutator. Further developments in high-power semiconductor electronics led to the introduction of the frequency–voltage conductor. As a consequence, the DC motors on diesel locomotive are currently replaced with polyphase brushless AC motors controlled by inverters. This not only decreased the maintenance even more (by eliminating the need of brush commutators as for the DC motors) but also enhanced the efficiency in variable traffic and load conditions.

The regulation of diesel-electric prime mover is well developed, although it is relatively complex. It is primarily done by adjusting the fuel rate which will influence both the torque and the rotational speed of the engine. The regulating governor reacts according to the fuel throttle setting and the rotational speed of the engine. Only the throttle can be adjusted by the locomotive driver. The power output, that is, the product of angular speed and torque, is independent on the road speed within the design limits for voltage and current of the alternator, but the torque—or the traction force—tends to decrease at higher speeds. Therefore, the generator is designed to produce low current and high voltage at high running speeds and low voltage and high current at low running speeds.

Initial diesel locomotive systems had a continuous (or analogue) mechanism for throttle adjustment. The control system included a governor and a load regulator. The governor mechanisms read two signals, namely the signal carrying the actual engine speed and that carrying the set point for the speed imposed by the locomotive driver. Based on these two signals, the governor determines the position of the throttle and the adjustment of the load regulator. In turn, the load regulator sets the excitation level of the alternator coils according to the signal received from the governor. The load generator acts as a variable electrical resistance which adjusts the voltage applied to the excitation coil of the generator. In fact, the coupling diesel engine and the alternator are made possible through the regulation of the excitation coil so that the electrical power generated matches continuously the mechanical power produced by the diesel engine. The mechanical power developed by diesel engine depends on the fuel rate and the rotational speed. The electrical power generated by the alternator is related only on the magnetic excitation level and is independent on the rotational speed. This is why the governor must adjust simultaneously the fuel throttle and the load regulator so that the mechanical power is fully transmitted to the generator and thence converted into electrical power.

If the rotation speed of the prime mover is too high, an alarm is produced which will cut the fuel supply to the engine. With this mechanism, the notches are changed sequentially and the jump over consecutive notches is not possible. The analogue control proved to be a difficult control system when multiple locomotive units are put to work together to haul a line train. Therefore, this system evolved into a digital one in which the fuel throttle is controlled in steps, also known as “notched” throttle control.

An electromechanical servomechanism is installed, which reacts on digital signals from the driver and adjusts the throttle in 9–10 notches. The jump over notches are possible due to a sophisticated control that modulates the signals for a smooth transition. Among the notches, one is the idle (when the throttle is set to minimal fuel for low rotation sped) and one is the emergency stop for shutting down the engine. During the idle mode, the alternator is electrically shut down by disconnecting the stator winding excitation such that power is not generated. Also, the electrical motors for traction are electrically decoupled from the alternator when the prime mover is in the idle mode.

Remote control is used in such a way that through a single electric cable, the same digital system is transmitted to all locomotive units of a line-haul which therefore will adjust the throttle exactly in the same way. The electric cable for transmitting the digital signals for the prime mover control needs to have only 4 wires to transmit 4 binary digits, which allows for a maximum of 16 throttle positions. The current diesel-electric locomotive movers are computer controlled. The data acquisition and computer system are programmed such that it compares at any time the power generated by the engine and by the alternator. For given engine notches, the computer system adjusts the alternator windings to match the prime mover and generator powers according to the settings from the operator. Another way of engine regulation is through the electronic fuel injection system, when applies.

The electric motors are regulated through voltage—as for DC motor case (nowadays obsolete, except for specific cases), or by frequency and voltage—as for AC electric motors. The electric motor regulation is quite complex. During the start-up, there is no rotating magnetic field produced since the shaft is not turning or is turning slow. Therefore, the current is limited by a low resistance and no reactance. As a consequence, the current is the maximum though the motors are rotating slowly. Since the torque is proportional to the current, the torque becomes maximum at start-up. If the wheels’ rotation sped increases due to acceleration, the motor winding starts to develop reactance, which diminishes the current and increases the voltage over the coil. Since the current diminishes, this does also the torque, but the revolution speed is high such that the power is constant. Eventually, the torque reaches a plateau corresponding to a traction force which balances the frictions. This situation leads to no net force and no acceleration; therefore, the current and voltage and the speed remain constant.

The starting process of a diesel-electric locomotive is described as follows:

- The direction is set by shifting a handle which will determine the modality in which the motors are connected such that they will turn either forward or in reverse.
- The throttle is moved to the first level simultaneously with releasing the brake.
- Connection of the generator and of the traction motors to the electronic blocks.
- Connection of the excitation coils of the alternator to the electrical circuit to produce magnetic field excitation and hence to start the generator.
- The locomotive (and the pulled train) starts to move. The system produces at this moment—according to the design—the maximum torque possible. The force developed by this high torque can be of over 500 kN for freight prime movers, thus being capable to pull trains of more than 10 Mt.
- If the fuel rate is not sufficient to accommodate the required traction force, the engine tends to stall; therefore, if this happens, the throttle must be shifted gradually to higher notches. This will increase the generated power and therefore will accommodate with the required traction force.
- Once the throttle is high, the excitation power of the alternator must be increased such that it accommodates with a higher generated power.

The braking process uses the traction motors in reverse, namely as generators. This type of braking is effective for speeds higher than ~20 m/h, or otherwise pneumatic braking is applied. This process is done as follows:

- The excitation coils of the traction motors are supplied with power by connecting them to the generator.
- A set of electric resistances are placed on the roof of the locomotive.
- Once the motor coils are connected to the electric resistances, the motors start acting as generators.
- The power generated by the motors is dissipated by the electric resistors.
- The motors working as generator consume power from the wheels by imposing a torque which opposes their rotation.
- Therefore, a braking force is developed which decelerates the movement.

3.7 Electric Locomotives

The electric locomotive comprises an electromechanical system which is connected to overhead line and generate propulsion power though the help of multiple electrical motors. In some cases, a rail is used to transport electrical power to the locomotives. The electric locomotive is highly efficient—with efficiency higher than 90%—because they do not incorporate engines. Rather, electrical power is converted to mechanical power directly. Emission of atmospheric pollutants therefore is eliminated.

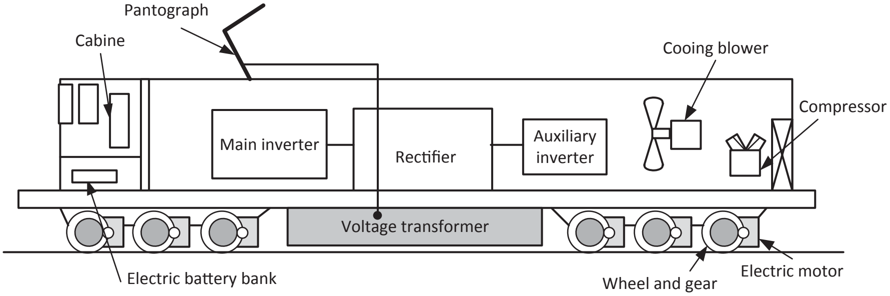


Fig. 3.9 Electric locomotive diagram

Furthermore, electric locomotive is very adapted for regenerative braking using inverter–AC motor, acting as power generators when braking is applied, being able to deliver power back to the line. The capital of an electrified line is higher than on regular railways, but the long-term economic benefit justifies the investment, especially for highly used railways and for high-speed trains.

Figure 3.9 shows the layout of an electric locomotive. The pantograph connects electrically to the overhead power line through a sliding mechanism. On the roof, a circuit breaker is placed. Then, the line connects with the voltage transformer placed under the locomotive. The AC voltage after the transformer is rectified and the DC power transferred to the main inverter and to an auxiliary inverter. The main inverter generates controlled AC power to drive the traction motors, whereas the auxiliary inverter drives all other equipment.

The proof of concept of electric locomotive was demonstrated in 1890s in Switzerland using AC power. Other early tests were performed in New York and Baltimore areas. The trolley pole has been developed which is guided into the line with the help of a shoe. Further development included the pantograph and the bow collector. The pantograph uses a hinged frame to press the shoe against the line. The bow collector glides a rod along the wire.

The initial designs of electric locomotives used large electric motors installed on the body of the locomotive and the mechanical power transmitted to the wheels via a jackshaft system and gears. Latter, quill drives were used for power transmission instead jackshafts. This system became obsolete with the development of more compact electrical motors that are capable of direct coupling with the wheels. This reduces the system complexity and the amount of maintenance required.

The axle-hung traction motors are now the norm on electric locomotives having one motor for each driven axle. A spur gear assembly is used to transfer power from the motor to the axle coupled by a pinion and a bull gear. A transmission casing encloses the gear system and the lubrication system. The transmission ratio of the gearbox differs depending on the type of operation. For passenger and commuter operations characterized by high-speed transportation, the gear ratio must be low, whereas for freight transport—with smaller speeds and higher tonnage—the transmission ratio is typically high.

3.8 Alternative Prime Movers

Several alternative locomotive prime movers exist for specific applications. As such, we have the biodiesel locomotive, hydrogen fuel cell locomotive, natural gas locomotive with various versions, namely liquefied or compressed natural gas in internal combustion engine and gas turbine configurations, battery electric locomotives, hybrid locomotives, and high-speed trains. Ammonia locomotives emerged as a potential transition option as detailed within this book.

As reviewed in [34], battery powered and battery hybrid locomotives have been operated primarily in switcher operations. Railpower technologies manufactured "Green Goat" diesel–battery hybrid switcher locomotives, on the recycled frames of retired locomotives. In 2001, the 2000 hp "Green Goat" prototype units entered service, followed by the smaller 1000 hp "Green Kid" prototype unit in 2003. Railpower manufactured production units from 2004 to 2006. The hybrid technology uses diesel gen-set(s) to recharge batteries and provides additional power as required, with overall fuel reduction of over 50 % in operational units.

Another use for battery locomotives is in industrial facilities where a combustion-powered locomotive (i.e., steam- or diesel-powered) could cause a safety issue, due to the risks of fire, explosion, or fumes in a confined space. Battery locomotives are preferred for mines where gas could be ignited by trolley-powered units arcing at the collection shoes, or where electrical resistance could develop in the supply or return circuits, especially at rail joints, and allow dangerous current leakage into the ground.

In 2009, Norfolk Southern, in collaboration with Penn State University and other industry partners, began demonstration of a 1500 hp EMD GP38 battery-powered locomotive for switcher operations in the Altoona, PA switchyard. The diesel prime mover and fuel tank were replaced with 1080 12 V lead-acid batteries, which power the locomotive throughout the day and are charged overnight. The locomotive uses regenerative braking to recharge the batteries during operation. To address issues such as overheating and burning, the battery management system and structural design have been optimized to improve battery maintenance and maximize battery life, and more advanced lead-carbon batteries, produced by Axion Power International, are being used in the current (2013) generation model of the battery-powered locomotive.

In 2003, General Electric (GE) tested a diesel–battery hybrid prototype locomotive for line-haul operation. The 4400 hp locomotive was powered by the diesel engine, with large capacity batteries storing up to 2000 hp equivalent, for up to 30 min. The project is being evaluated for its practicality and commercial viability—the large size of the batteries makes locomotive maintenance difficult, requiring an entire side of the locomotive for the battery bank.

3.9 Closing Remarks

In this chapter, the main types of prime mover for locomotives are reviewed. A historical perspective is given on the locomotive prime mover evolution. Then, the steam locomotives, diesel locomotive, diesel-electric locomotive, electric locomotive, and some alternative systems are explained based on their operational and technical aspects as well as their advantages and disadvantages.

Chapter 4
Potential Fuel Options

4.1 Introduction

Transportation fuel alternatives are an active area of research and development with many complex factors affecting the progress of potential options, from technological advances and challenges to environmental considerations, energy security concerns, and public perception.

There are numerous and significant reasons to implement more benign transportation fuels in place of traditional fossil fuel-derived hydrocarbons; these resources are finite, with significant environmental, human health, and sociopolitical implications resulting from their extraction and combustion. However, fossil fuels are highly practical and have high energy density that makes them particularly suitable for transportation. Furthermore, advances in vehicle and fuel technologies have generally gone hand in hand—imposing a considerable bias in their favor that is difficult for less mature alternatives to overcome in the short time frame that is necessary to effectively slow the rate of nonrenewable resource depletion and climate change.

The challenge at hand is to provide alternatives with sufficient energy content and lower environmental impact that are comparable in terms of availability, practicality, and economics. Potential fuel options for clean rail applications including natural gas (NG), synthetic and biodiesel fuels, hydrogen (H_2), and ammonia (NH_3) are discussed in the following sections. The status of resources and technologies are briefly given for each, and comparisons are made regarding various physical, environmental, and economic factors.

I. Dincer et al., *Clean Rail Transportation Options,* Green Energy and Technology,
DOI 10.1007/978-3-319-21726-0_4

4.2 Conventional Transportation Fuels

Diesel and gasoline transportation fuels dominate for both light- and heavy-duty vehicles and—until recent years—have remained largely unrivaled in this respect. In 2012 data for medium- and heavy-duty vehicles in the USA, diesel engines represented 99.4 % of registered vehicles and 94.7 % of diesel fuel consumption [35]. Gasoline vehicles are primarily light-duty vehicles, such as passenger cars and light-duty trucks.

The lack of diversity in transportation fuel options has certain advantages and disadvantages; technologies and infrastructures for diesel and gasoline fuels are mature, well understood, and economic relative to most alternatives. However, without major competition to maintain cost control, the fuel prices fluctuate significantly. Figures 4.1 and 4.2 show historical prices for gasoline and diesel fuels for several developed and developing countries, and the world average.

Generally speaking, the pump price of diesel fuel has been lower than that of gasoline, but with recent fuel regulations to reduce the amount of sulfur, soot, and other pollutants increasing the cost of processing, diesel fuel price exceeds gasoline by an average of 9.2 % since January 2012 [35]. The higher efficiency of diesel engines partially offsets this increase, but is still a strong motivating factor for the implementation of more economic alternatives in large diesel engines such as locomotives.

Crude oil reserves are another pressing issue to be taken into consideration, in terms of both resource depletion and the effect of increasing demand on fuel pricing. In 2010, proven recoverable domestic crude oil reserves in the USA totaled 25.2 billion barrels, and 2.0 billion barrels were extracted [38]. At this rate, there is only a 13-year supply remaining, although new crude oil discoveries and extraction methods suggest total proven and unproven reserves of up to 219 billion barrels in the USA as of 2011 [38]. Population growth and improved standards of living will

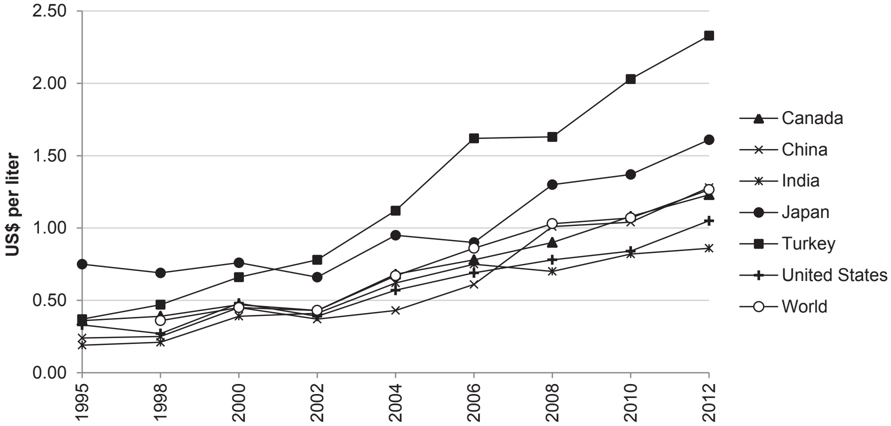


Fig. 4.1 Pump prices for gasoline. (Data from [36])

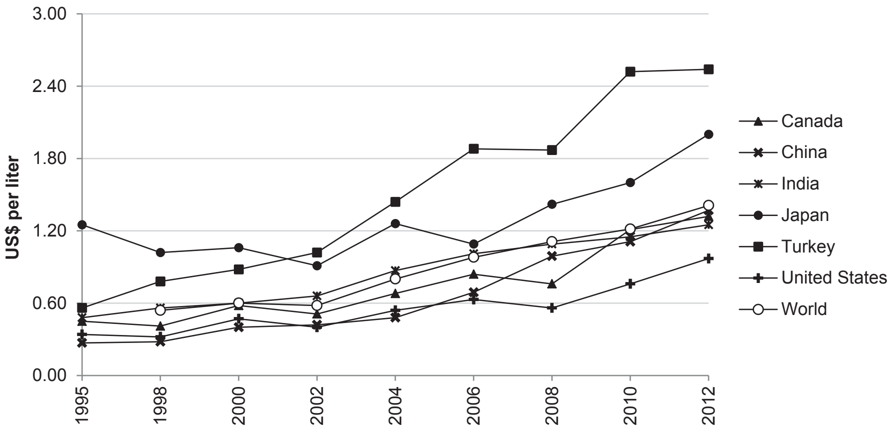


Fig. 4.2 Average pump prices for diesel fuel. (Data from [37])

continue to increase the demand, and costs of petroleum fuels may reach a prohibitive level for many applications over the next 45 years [38, 39].

4.3 Natural Gas (NG)

NG is at the forefront for alternative transportation fuel implementation, with compressed and liquefied natural gas (CNG and LNG) gaining usage in heavy-duty vehicle applications such as rail and transit buses. The majority of NG composition is methane (CH_4), which produces lower levels of GHGs in its combustion than diesel or gasoline, has approximately the same fuel economy as a gasoline engine, and is low cost. Most NG extraction is from well stations or as part of crude oil extraction processes.

NG is a fossil fuel with finite supply; however, advances in shale gas extraction technologies have led to an increase in proven recoverable resources, seen in by global and regional trends, Fig. 4.3, and a likewise increase in estimation for the supply lifetime for NG. An estimate of 100-year supply of domestic NG in the USA based on current reserves and technologies is given by [40].

Hydraulic fracturing (fracking) techniques extract shale gas held in subsurface reservoirs of porous rock. Horizontal drilling technologies have made it possible to extract significantly more shale gas than vertical well drilling alone. In the fracking process, wells are drilled into shale rock to depths reaching nearly 3000 m, where the drilling then extends horizontally. Millions of liters of a slurry, mixture of water, chemicals, and sand, are then pumped at high pressure into the drilled pathways, which fractures the shale. Gases escape from the rock formation through these fractures—held open in tiny amounts by sand particles lodged during the pumping process—and flow out of the well where collection and refining can take place. While

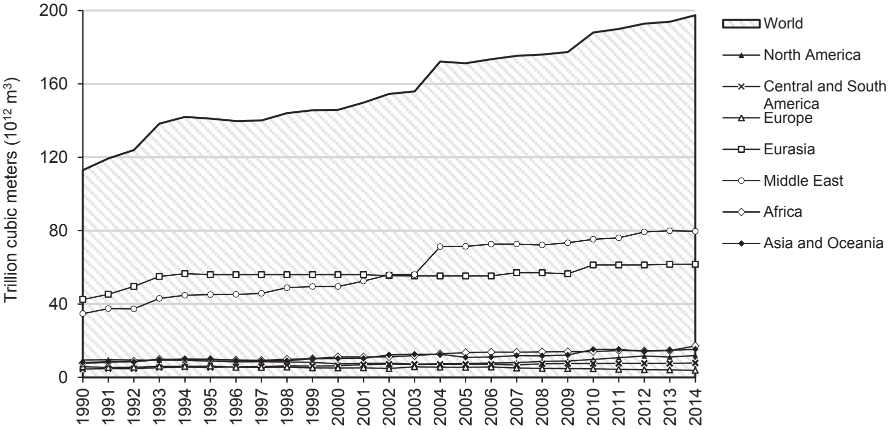


Fig. 4.3 World and regional proven natural gas reserves. (Data from [41])

this method greatly extends the availability of NG, there is significant resistance to this technology due to unknown environmental effects of the process, such as fracking slurry chemicals and methane (shale gas) seeping into watershed bodies and drinking water supplies [38].

In CNG vehicle applications, the gas is stored at pressures of 20–25 MPa and less than 1 % of its volume at STP LNG requires energy-intensive cooling equipment to maintain a temperature below − 160 °C needed to remain in a liquid phase. Both NG options require expensive storage equipment—approximately $95/L for CNG, and $125/L for LNG—as well as other engine modifications to operate with gas fuel in place of liquid. This is offset in part by the low cost of NG (Fig. 4.4), which is low cost in comparison with diesel fuel.

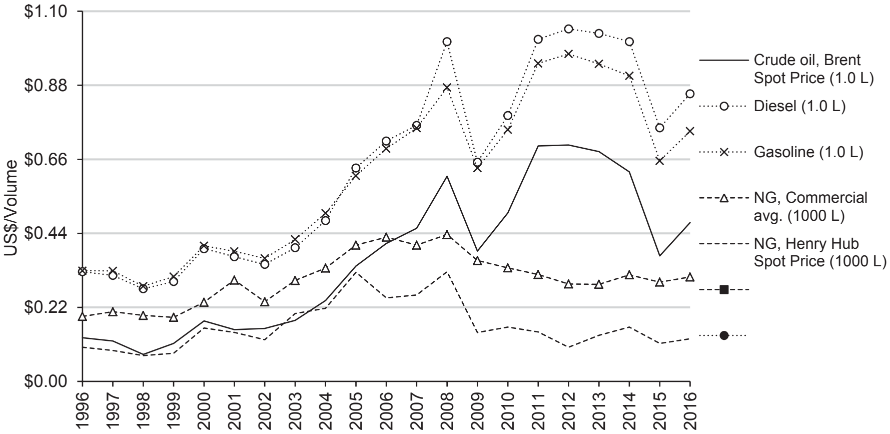


Fig. 4.4 Fuel prices and 2016 projection for petroleum and natural gas fuel options. (Data from [41])

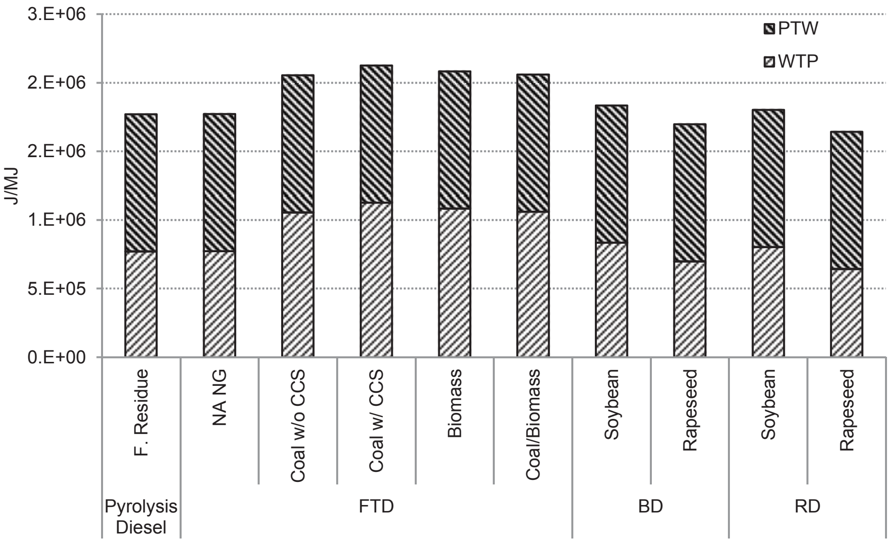


Fig. 4.5 Energy demand for production and transportation biofuels and synthetic fuels for different methods. (Data from [42])

Continuing progress in NG extraction processes and fueling technologies suggest that CNG and LNG fueling will have a significant role in the shift away from petroleum fuels. Furthermore, it is possible to produce renewable NG using biomass making fossil NG a good transition fuel toward sustainable and renewable fuel options.

4.4 Biofuels and Synthetic Hydrocarbon Fuels

Fischer–Tropsch conversion, gasification, and fast pyrolysis processes produce synthetic fuels from feedstocks such as NG, coal, and biomass. In the Fischer–Tropsch process, synthetic hydrocarbons are produced over metal catalysts at high pressure. Pyrolysis uses very high temperatures to produce bio-oil, which is then hydrotreated to composition of renewable biogas that can be converted to synthetic natural gas (SNG) and renewable diesel (RD) fuel. These fuels are compared in terms of energy demand in Fig. 4.5 for several methods using the GREET software package from [42].

4.5 Hydrogen

Hydrogen (H_2) is widely accepted as the ideal fuel for sustainable development, with the highest gravimetric energy content and no harmful pollutants resulting from its combustion. The primary method of producing H_2 is through steam-meth-

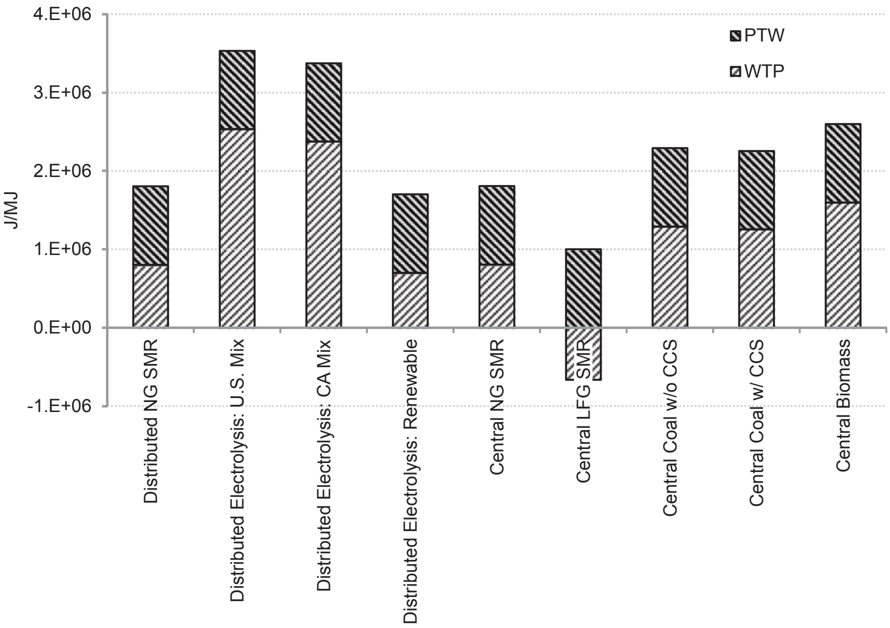


Fig. 4.6 Energy demand for production and transportation of H_2 fuel for different methods. (Data from [42])

ane reforming (SMR) of NG, though synthetic NG options offer a transition toward more sustainable options as renewable energy resources gain maturity.

The energy requirement for various hydrogen production methods are shown in Fig. 4.6 using GREET software to plot the total energy requirements based on various feedstocks. These are later considered in the GHG comparison of the potential fuel options.

Before the realization of a hydrogen economy, there are challenges that require innovative solutions. The first, and most significant, is development of efficient storage methods; hydrogen is the lightest element and requires either large volumes, high pressure, low temperature, or advanced material storage techniques to hold sufficient fuel for practical operating range [43]. The characteristics of the main storage options are given in Table 4.1.

Table 4.1 Comparison of hydrogen storage methods. (Source: [44])

Storage method	Energy intensity (MJ/kg-H_2)	wt%-H_2/tank	wt%-H_2/kg-system	g-H_2/tank	g-H_2/L-system
Compressed H_2 (35 MPa)	10.2	6	4–5	20	15
Liquid H_2	28–45	20	15	63	52
Low temperature hydrides (T < 100 °C)	10–12	2	1.8	105	70
High temperature hydrides (T > 300 °C)	20–25	7	5.5	90	55

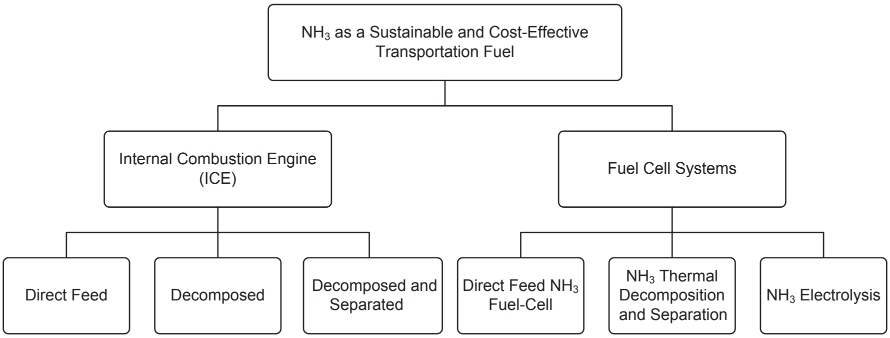


Fig. 4.7 Ammonia fueling applications. (Reproduced from [46])

4.6 Ammonia

Ammonia has been considered for alternative fueling in transportation applications for more than 70 years [45] and is an important nitrogen source used in agricultural and industrial applications. There are two possible pathways for NH_3 as a transportation fuel: ICE engines and fuel cell systems, with the subcategories for each application indicated in Fig. 4.7. The present focus is ICE applications for NH_3 fuel, with the alternative locomotive configurations integrating direct feed or a combination of direct feed and decomposition subcategory options for NH_3 fuel utilization.

Ammonia has many qualities that highlight it as a sustainable alternative to hydrocarbon fuels for transportation applications. Based on a review of multiple studies by [46] on the potential of ammonia as an alternative transportation fuel, the following are emphasized as particularly advantageous qualities of NH_3:

- High octane rating of NH_3 (110–130) makes it suitable for ICE applications [47]
- With more than 150 Mt produced internationally each year, there is already a well-established production and distribution infrastructure in place for NH_3
- Can be thermally decomposed into H_2 for fuel, and N_2 gas
- NH_3 is safer than other fuels, including hydrogen, due to high rate of dissipation in air, strong (self-alarming) odor at very low concentration (~5 ppm in air), and is considered nonexplosive due to its very narrow flammability range.

The thermophysical properties of ammonia are listed in Table 4.2. The high latent heat of vaporization, in particular, makes it a useful working fluid to provide indirect engine cooling, and can reducing the demand on the engine-driven cooling systems by providing indirect cooling of water coolant streams. Recovered heat may be utilized in various NH_3-based processes, producing additional power, and/or heating and cooling applications (refrigeration, cabin air conditioning).

Ammonia is formed from two of the most abundant chemical elements in the universe—hydrogen and nitrogen—and is most commonly produced using the Haber–Bosch process, combining hydrogen and nitrogen in the reaction:

Table 4.2 Thermophysical properties of ammonia. (Source: [48])

Molecular formula	NH_3
Molecular weight, M_i (kg/kmol)	17.03
Liquid density, ρ (kg/m^3) (T=25 °C, P=101.3 kPa)	603
Vapor density, ρ (kg/m^3) (T=0 °C, P=101.3 kPa)	0.888
Critical pressure, P_{cr} (MPa)	11.28
Critical temperature, T_{cr} (°C)	132.4
Latent heat of vaporization, h_{fg} (kJ/kg)	1370
Standard enthalpy of formation, h^o (T=25 °C), (kJ/kmol)	−46.22
Standard entropy, s^o (T=25 °C, P=101.3 kPa), (kJ/kmol·K)	192.7
Lower heating value, *LHV* (MJ/kg)	18.57
Higher heating value, *HHV* (MJ/kg)	22.54
Chemical exergy, ex^{ch}	19.84

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

Hydrogen required for the reaction is obtained by the electrolysis of water or fuel reforming to generate synthesis gas. The most common NH_3 production methods are compared briefly in Table 4.3. GHG emissions from ammonia production with fuel reforming are associated with either fuel combustion or process-related CO_2 emissions; fuel-related emissions result from combustion of CH_4 for steam/gas reforming and various heat requirements, and process-related CO_2 emissions result from the conversion of NG (CH_4) to H_2 and CO_2 during synthesis. Many facilities producing ammonia recover a portion of CO_2 to produce urea, helping to reduce the overall GHG emissions and improve sustainability, while producing an additional valuable product.

NG is the primary feedstock used for producing ammonia in Canada and worldwide. There are 11 ammonia plants operating in Canada, producing an average of 4–5 Mt annually per plant [49]. Canadian ammonia plants recover a high percentage of process-generated CO_2 (~40 %) to produce urea and have the highest feed-plus-fuel energy (FFE) plant efficiency internationally [49]—consuming an average of 33.8 GJ/t-NH_3 for NG plants, compared to the international average of 38.6 GJ/t-NH_3.

In 2014, worldwide production of anhydrous ammonia was 175 Mt [53], with the highest ammonia production by China at 58.4 Mt. The production capacities of selected developed and developing countries are shown in Fig. 4.8 as a percentage of total production. According to [53], global ammonia production is expected to see further growth of 16 % by 2019, primarily in China.

Given that the primary energy resource for NH_3 production is NG, it is valid to propose to simply use NG directly for transportation fuel application—skipping the middle man so to speak—but this does not take into account several key factors that make NH_3 an attractive option for sustainable development:

Table 4.3 NH_3 production method comparison[a] (intensities per tonne NH_3). (Sources: [45, 50–52])

Production method	Fuel	Energy (GJ/t)	Emissions t-CO_{2eq}/t	\$/t	Details
SMR	Natural gas (CH_4)	38.6 (33.8[b])	1.8	400–1000	Most common method Fossil fuel derived Highly unstable price
Gasification	Coal	54	4.6		Predominantly used in China High energy and emission intensity
H_2O electrolysis	Electricity (hydro)[c]	12 GWh	–	255–735	Electricity may be produced from renewable and nonrenewable resources
Solid-state ammonia synthesis (SSAS)	Electricity (hydro)[c]	7.5 GWh	–	140–440	Proton conducting membrane reactor eliminates need for electrolyzers and Haber–Bosch process Co-production of O_2 Direct steam to NH_3

[a] Haber–Bosch process for NH_3 synthesis for all except SSAS
[b] Canadian average
[c] Electricity from 1 to 5 ¢/kWh

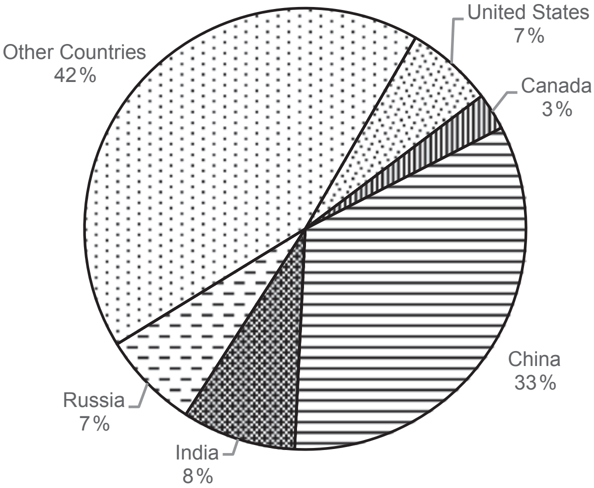


Fig. 4.8 Ammonia production capacity by country, 2014. (Data from [53])

- NH_3 is naturally occurring in biological systems and does not do harm to the environment or human health in low quantities; it is necessary in agriculture to fertilize food crops.
- NH_3 is not a fossil fuel and therefore is not finite to fuel reserves, which will eventually be completely depleted.
- NH_3 can be produced entirely from renewable resources and does not require energy and environmentally taxing extraction processes to be made available.
- NH_3 does not contain any carbon and therefore does not produce and CO_2, CO, or soot (a primary constituent of particulate matter) during combustion.
- Currently and historically used in a multitude of applications from nitrogen-rich fertilizer, to household cleaner, refrigerant, NOx emission reduction agent, and fuel.
- Storage of ammonia is similar to that of liquid propane and is able to be stored as a liquid under mild-pressure conditions (~ 1000 kPa).

With one of the highest production rates of any chemical, there is a very well-established transportation and delivery infrastructure in place for NH_3, both nationally and internationally, using rail, marine, truck, and pipeline transport methods. It is also possible to produce ammonia locally (relative to fueling points) from renewable sources, which can give further reductions in CO_2 emissions by minimizing the environmental and impact of transporting ammonia and, most significantly, can eliminate (or nearly eliminate) the feedstock-related emissions. Biofuel and biomass offer a sustainable option for ammonia production, for both syngas production and as a fuel for power plants to produce electricity for water electrolysis. Furthermore, biofuels may be produced locally from various agricultural feedstocks and/or waste, and municipal solid waste.

4.7 Summary and Comparison of Conventional and Alternative Fuel Options

The various energy, environmental, and economic characteristics of the potential fuel options are summarized in side-by-side comparisons of the fuels. Various thermophysical and combustion properties are listed in Table 4.4. These values give an overview of certain parameters that help identify which fuels are of most interest for a given application. For the case of rail transportation considered in this book, it is clear that those fuels most closely resembling the properties of diesel are good candidates, for example, biodiesel B100, while fuels that require extreme storage conditions present a challenge for long-haul rail transport.

Comparison of the energy densities of traditional and alternative fuels is shown in Fig. 4.9. Although the low-volumetric energy density of ammonia, relative to traditional hydrocarbons, presents a challenge to its introduction in passenger vehicles as a direct feed combustion fuel—requiring more than double the volume of diesel fuel or motor gasoline to provide the same amount of energy—large transportation

Table 4.4 Thermophysical and combustion properties of fuel options. (Source: [46, 55])

Property	Gasoline	ULSD	CNG	LNG	B100	Hydrogen	Ammonia
Feedstock	Crude oil		NG reserves, biogas (SNG)		Soy, waste oil, fats	NG, H_2O electrolysis	NG
Molecule	C_8H_{18}	$C_{12}H_{23}$	CH_4	CH_4	$(C_{12}–C_{22})$	H_2	NH_3
Physical state	Liquid	Liquid	Comp. gas	Cryogenic liquid	Liquid	Comp. gas or liquid	Liquid
HHV (MJ/kg)	46.7	45.5	42.5	50	40.1	5.7	22.5
Storage density (kg/m_3)	736	850	188	450	880	10 ($H_{2,g}$) 70.8 ($H_{2,\ell}$)	603
Storage pressure (bar)	1	1	20–25	~8	1	200–500	10
Cetane number	–	40–55	–	–	48–65	–	–
Octane number	84–93	–	120+	120+	–	130+	110–130
Flash point (°C)	−43	74	−184	−188	100–170	–	–
Autoignition temperature (°C)	257	225	540	540	150	565–585	651
Ignition limits (vol% in air)		0.6–5.5	5–15	5–15		4–75	16–25

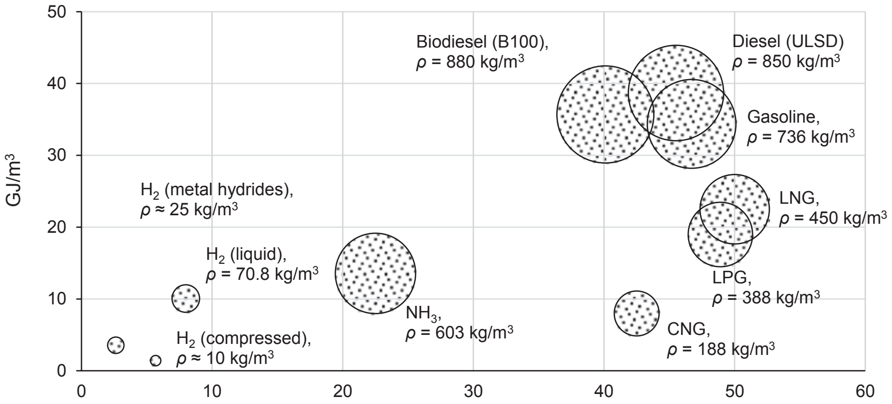


Fig. 4.9 Volumetric (GJ/m^3) and gravimetric (GJ/t) energy density, and mass storage density (kg/m^3) of transportation fuels [46]

vehicles such as rail and heavy-duty trucks are well equipped to carry the additional fuel weight without prohibitive performance penalties.

One of the most immediate factors to consider in comparing fuel alternatives is their potential reduction in high levels of greenhouse gas and other emissions hazardous to environment and health. The carbon–hydrogen ratio of various transportation fuels is shown in Fig. 4.10. Although biodiesel (B100) has a similar carbon content as petroleum diesel, this content is largely neutral in combustion depend-

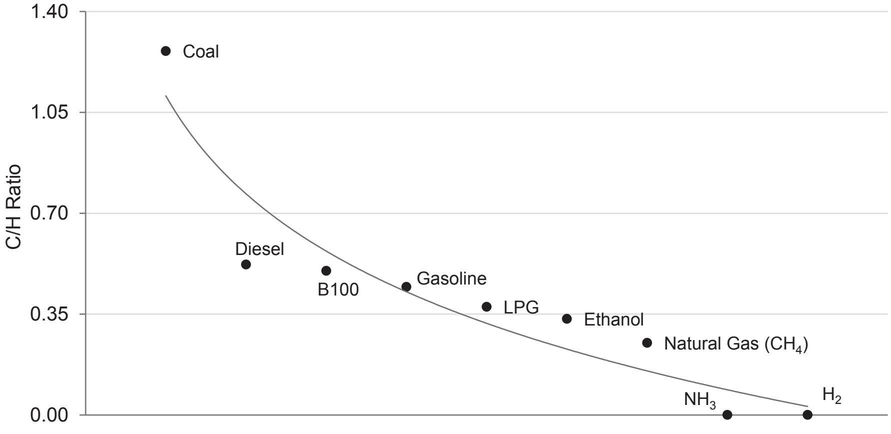


Fig. 4.10 Carbon/hydrogen ratio of common transportation fuels

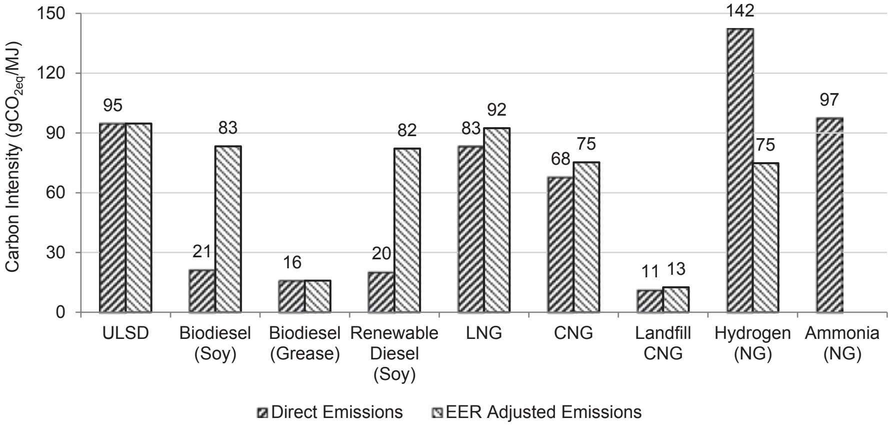


Fig. 4.11 Direct and energy economy ratio (EER)-adjusted carbon intensity of fuels for heavy-duty vehicles. (Data from [55])

ing on the feedstock. Compared to other fuels used in combustion applications, ammonia has the highest hydrogen energy density—higher even than pressurized and liquefied hydrogen fuel, based on current storage methods [47]—contains no carbon, has a global warming potential (GWP) of zero, and produces only nitrogen and water when combusted.

It is important to consider not only the amount of carbon in the fuel composition that will be converted to GHGs during combustion, but also the carbon intensity of the fuel itself and how efficiently the fuel is utilized. Figure 4.11 plots the carbon intensities for direct emissions based on fuel feedstock, as well as the adjusted value based on the energy economy ratio (EER) of each fuel for combustion in a heavy-

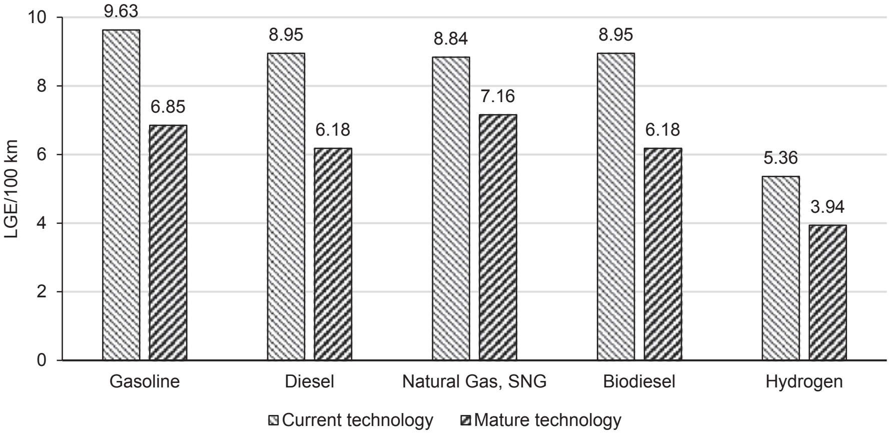


Fig. 4.12 Light-duty vehicle fuel economy comparison by fuel. (Data from [56])

duty vehicle engine. This EER-adjusted value is not included for NH_3 and only considers the direct carbon emission intensity for typical NG feedstock.

As a practical measure of comparison, fuel economy of light-duty vehicles is shown in Fig. 4.12 based on current fuel technologies and estimates for mature technology scenarios. The values are given in terms of liters of gasoline equivalent per 100 km driving range (LGE/100 km), and indicate that with sufficient research and development for alternative fuels technologies, these options can meet or exceed gasoline and diesel fuels in terms of fuel economy. GHG emissions for the various life cycle stages are compared in Fig. 4.13 for well-to-pump (WTP), pump-to-wheel (PTW), and total well-to-wheel (WTW), using GREET software. These show the advantage of utilizing biomass resources to reduce the environmental impact of fuels, and also the demand on nonrenewable resources.

When considering potential transportation fuels for public use, possible physical and chemical hazards require careful consideration in order to maintain safe operation of transportation vehicles and fueling stations. Ammonia is classified as a toxic substance, with a low risk of flammability.

Compared with the health and flammability ratings of other fuels in Fig. 4.14, the flammability risk is significantly lower than NG fuels and hydrogen, which are considered explosive and are also stored at much higher pressures than NH_3. While NH_3 does have toxic properties, one must be exposed for an extended period of time at high local concentrations of NH_3 before it becomes a significant health risk. Furthermore, NH_3 has a very strong and pungent odor at very low concentrations, thus providing ample warning to leave an area if a leak should occur. Furthermore, while hydrocarbons are not necessarily cancer causing in their fuel form, their combustion products are identified as a cause of lung cancer by health organizations such as the WHO and Canadian Cancer Society [57, 58].

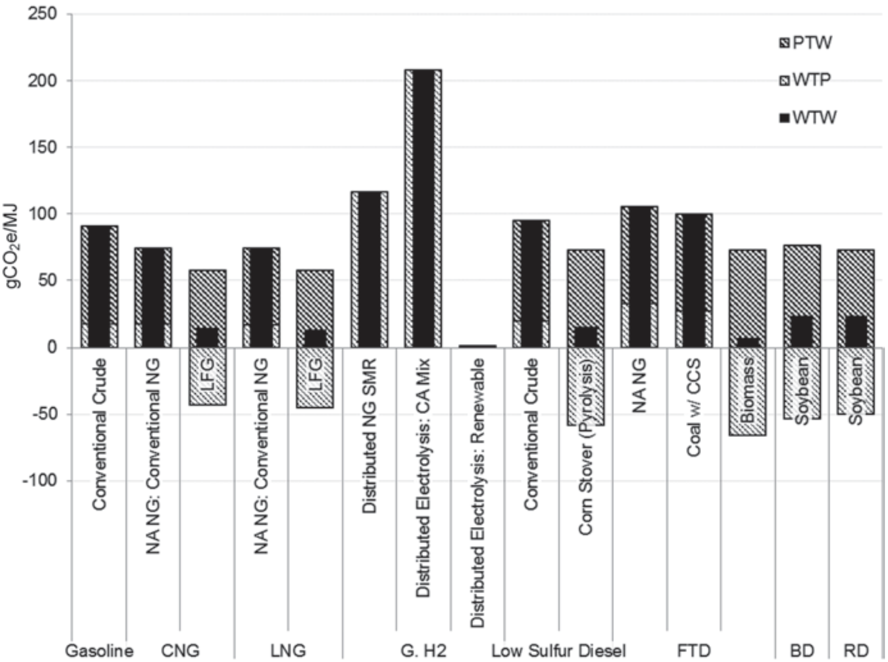


Fig. 4.13 Greenhouse gas emissions for potential fuel options for life cycle stages. (Data from [42])

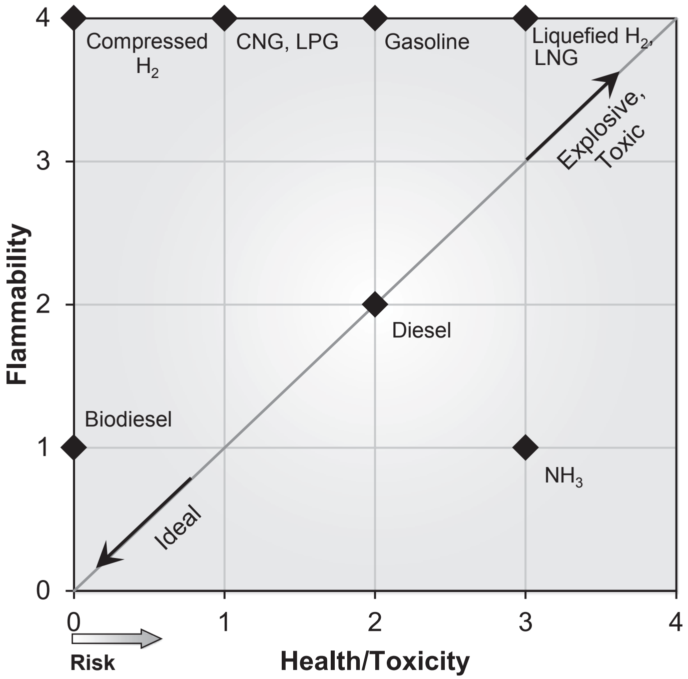


Fig. 4.14 Toxicity and flammability of common transportation fuels. (MSDS from [59])

4.8 Closing Remarks

Potential options for clean transportation fuels are necessary for meeting climate change goals and preserving finite energy resources. The various fuel options that may act as transition fuels toward sustainable and renewable fuel options appear to be NG—which can be produced synthetically from biogas—and ammonia, which can be produced from any electricity source or renewable NG as these technologies mature. Considering options that are able to adapt to renewable production methods and domestic feedstocks, it is possible to set a path toward sustainable future and better energy security while also preserving nonrenewable resources for future generations.

Chapter 5
Clean Rail Initiatives

5.1 Introduction

Utilization of any kind of energy resources leads unavoidably to some environmental impact. However, if one succeed to increase the energy conversion efficiency of systems and processes then a reduced environmental impact can be achieved. Higher efficiency means less resource utilization and therefore, less associated pollution.

Realizing the importance of air pollution reduction in railway transportation, many governments and organizations have on their agenda clean rail initiatives. The problem is complex due to the large scale of railways with important air emissions due to two types of sources: (i) diesel engines on locomotives and (ii) power plants producing energy for electric locomotives. Ad hoc consortia of rail operators and research can be remarked for some instances.

The clean rail initiative referred in majority to the amelioration of the emission characteristics of diesel fuel, which is the most used to propel train locomotives. Many programs focus on the implementation of selective catalytic reduction systems on locomotives. Using various diesel blends such as diesel/biodiesel is also an option much considered in the past.

One of the most prominent clean rail initiatives is the introduction of hydrogen trains. Much research is devoted to this subject, and also, governmental projects using public or public/private funding can be remarked. As an alternative to hydrogen economy, one has the methanol economy which will be discussed subsequently. Thenceforth, certain research and funding initiative, although comparatively small, is remarked for methanol locomotives. Moreover, ammonia locomotives were also proposed as an alternative to the hydrogen economy.

One major research segment and funding is on natural gas locomotive, either as compressed gas or as liquefied methane. Pilot projects were developed in the past

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few decades to cover these alternatives to clean rail, as natural gas is much cleaner than diesel with respect to emissions, especially the GHG release per kW of shaft power.

In this chapter, the relevant worldwide clean rail initiatives are reviewed. Hydrogen, methanol, and ammonia economy concepts are introduced in this context. Development programs for reducing the emissions of diesel engines for locomotives and improvement technologies are presented. The major fuel alternatives discussed are biodiesel, hydrogen, natural gas, methanol, ammonia, and LPG. Also engine alternatives such as solid oxide fuel cells (SOFC) locomotive or gas turbine locomotive are discussed.

5.2 Hydrogen Locomotive Initiatives

The energy crisis from the beginning of the 1970s influenced positively the consideration by the scientific community of a hydrogen economy. In the initial views—characterizing the years of the 1970s—hydrogen stored in large scales would be transported at long distances (~ 1000 km) for which the economics shows that its transportation is better than electricity. In more recent years, another concept appeared, namely hydrogen storage at small scales, to satisfy power generation needs in vehicles or small power generators.

Using hydrogen as energy carrier can help reducing environmental damage and achieve sustainability. If hydrogen is produced from clean and renewable energy sources, the environmental impact is reduced, mainly through following facts: Fossil fuel resources are not consumed, and hydrogen combustion emissions do not contribute to global warming and do not generate substantial waste. At hydrogen utilization phase, the associated processes are more efficient than with traditional fuels. For example, fuel cell technologies can provide more efficient, effective, environmentally benign and sustainable alternatives to conventional energy technologies, particularly fossil-fuel-driven ones. Hydrogen energy systems are treated as a key component of sustainable development for four main reasons:

- They are compatible with renewable energy sources and carriers for future energy security, economic growth, and sustainable development.
- The variety of hydrogen and fuel cell technologies provide a flexible array of options for their use in various applications with reduced environmental impact and increased efficiency.
- Hydrogen cannot be depleted since the basic source is water. In contrast, fossil fuel and uranium resources are diminished by extraction and consumption.
- These technologies favor system decentralization and local and individual solutions that are somewhat independent of the national network, thus enhancing the flexibility of the system and providing economic and environmental benefits to small isolated populations.

Even if hydrogen is produced from fossil fuel sources, which normally cause burden on the environment, it is almost certain that hydrogen technologies can provide a cleaner and more sustainable energy system than increased controls on conventional energy systems. The key points can be stated based on the following facts:

- It can be converted from all traditional primary energy sources (coal, natural gas, and biomass) and, by using thermal energy and/or electricity, from all renewable energy sources and from nuclear energy (via electrolysis or various high-temperature technologies).
- It can flexibly be used in stationary and mobile applications without damaging emissions especially by using fuel cells.
- It can be made available everywhere and can potentially substitute oil and gas with no carbon-related emissions.

Hydrogen is only a secondary energy source (a "storage carrier") and must be produced from a primary energy source. Because of physical reasons, there will always be losses from these conversion processes, and therefore in any case, the costs of hydrogen must be higher than the costs of the energy used to produce hydrogen. This simple physical reason makes the decision on priorities and timescales for the introduction of hydrogen extremely complex. It is the same simple methodology leading to a higher CO_2-mitigation effect while using the input energy carrier for the production of hydrogen directly.

Some scientific and technical challenges for hydrogen economy may be given as follows:

- Lowering the cost of hydrogen production to a level comparable to the energy cost of petrol.
- Development of a CO_2-free route for the mass production of sustainable hydrogen at a competitive cost.
- Development of a safe and efficient national infrastructure for hydrogen delivery and distribution.
- Development of viable hydrogen storage systems for both vehicular and stationary applications.
- Dramatic reduction in costs and significant improvement in the durability of fuel cell systems.

The advantages of hydrogen versus fossil fuels can be listed as follows:

- Liquid hydrogen is the best transportation fuel when compared to liquid fuels such as gasoline, jet fuel, and alcohols; and gaseous hydrogen in the best gaseous transportation fuel.
- While hydrogen can be converted to useful energy forms (thermal, mechanical, and electrical) at the user end through five different processes, fossil fuels can only be converted through one process, i.e., flame combustion. In other words, hydrogen is the most versatile fuel.
- Hydrogen has the highest utilization efficiency when it comes to conversion to useful energy forms (thermal, mechanical, and electrical) at the user end. Overall,

Table 5.1 Worldwide associations which are active in hydrogen energy

Organization	Year[a]	Description
IAHE	1974	International Association of Hydrogen Energy is the main pillar in the hydrogen movement and its initiator. It governs the World Hydrogen Energy Conference and it is responsible for publishing the International Journal of Hydrogen Energy
ISO	1990	Formed 10 subcommittees to implement international standards for hydrogen energy technologies
NH_3FA	2003	Ammonia Fuel Association promotes ammonia as a source of hydrogen for better and more compact storage. It indirectly sustains a hydrogen economy. It started as a series of annual conferences since 2003, named the Annual Ammonia Alternative Fuel Conferences
CHFCA	2009	Canadian hydrogen and fuel cell association collaborates with IAHE to promote hydrogen adoption in Canada. It was formed in 2009 as a result of a merger of the Canadian Hydrogen Association (CHA) and hydrogen and fuel cells Canada. Through the former CHA, the CHFCA has been active in the field of hydrogen energy for over 25 years

[a] year since the organization became involved in hydrogen energy activities.

hydrogen is 39 % more efficient than fossil fuels. In other words, hydrogen will save primary energy resources. It could also be termed as the most energy conserving fuel.

- When fire hazards and toxicity are taken into account, hydrogen becomes the safest fuel.

A key event impacting the progress of the hydrogen economy concept was the THEME conference held in Miami (FL) in 1974. The International Association of Hydrogen Energy (IAHE) was established at that time, which became a world leader in promoting the hydrogen economy concept. One of the most known and prolific conferences—initiated and maintained by IAHE—is the World Hydrogen Energy Conference (WHEC), the first being held in Miami, 1976. By 2005, the Kyoto Protocol was signed, which represents an engagement of many countries to develop a cleaner energy system; hydrogen is an important part of this goal.

Table 5.1 contains a sample list of hydrogen associations worldwide. By the end of the 1980s, the hydrogen economy concept became well known. Russia started publication of Nuclear-Hydrogen Energy Technology periodicals showing a systematic scientific effort for developing a hydrogen economy from nuclear energy. By the end of the 1990s, many of the fundamental problems of hydrogen production, transportation, distribution, storage, utilization, materials, and safety were solved.

As a result of the sustained effort in promoting hydrogen—the future energy carrier—many governments initiated research programs on the topic. Some relevant clean rail initiatives of these programs are listed in Table 5.2.

These led to many accomplishments, some of them very spectacular like the first flight demonstration of a large-sized hydrogen passenger plane—Tupolev 155—in Moscow (1988), marketing of the first 1 MW SOFC with 70 % efficiency by West-

Table 5.2 Sample national or international hydrogen programs

Region	Program	Year	Description
WE-NET (Japan)		1993	"Clean Energy Systems Utilizing Hydrogen" is a program aiming to realize the "World Energy NETwork." The project term is 1993–2020
ARISE(Texas)		1990	NSF Center for H_2 research. Electrolysis and photoelectrolysis of H_2S to generate hydrogen. Photocatalysis of water
Freedom Car and Hydrogen (USA)		2005	DOE program to promote hydrogen economy in USA
Europe	Shell Hydrogen	2000	$500 M for hydrogen programs
	CUTE		Clean urban transport for Europe
	ECTOS	2000	Ecological city transport system
	Quickstart	2003	Hydrogen production from renewables to use and propel vehicles
	HyCHAIN	2006	Over 160 FC vehicles in Germany, Spain, and Italy.
Euro-Quebec (Canada–Europe)		1992	European–Canadian project to study the transport of hydropower from Quebec to Hamburg in the form of cryogenic hydrogen moved on barges
NRC–Vancouver (Canada)		2010	Around 10 hydrogen fueling stations were installed in Vancouver during the Olympic games
Cu-Cl cycle (Ontario)		2011	International consortium of 5 countries developing an integrated plant of the copper cycle of thermochemical water splitting for nuclear hydrogen production
HySolar (Germany–Saudi Arabia)		1986	Promoting hydrogen as an energy carrier for long distances. Development of hydrogen production methods
PAN'H (France)		2005	National Programme for hydrogen action
Iceland (Iceland)		1998	Aim to convert Iceland to a complete hydrogen economy by 2030
UNIDO-ICHET (Turkey)		2004	International center for hydrogen energy technologies formed as a UNIDO project funded by the ministry of energy and natural resources of Turkey with the role to promote the hydrogen economy

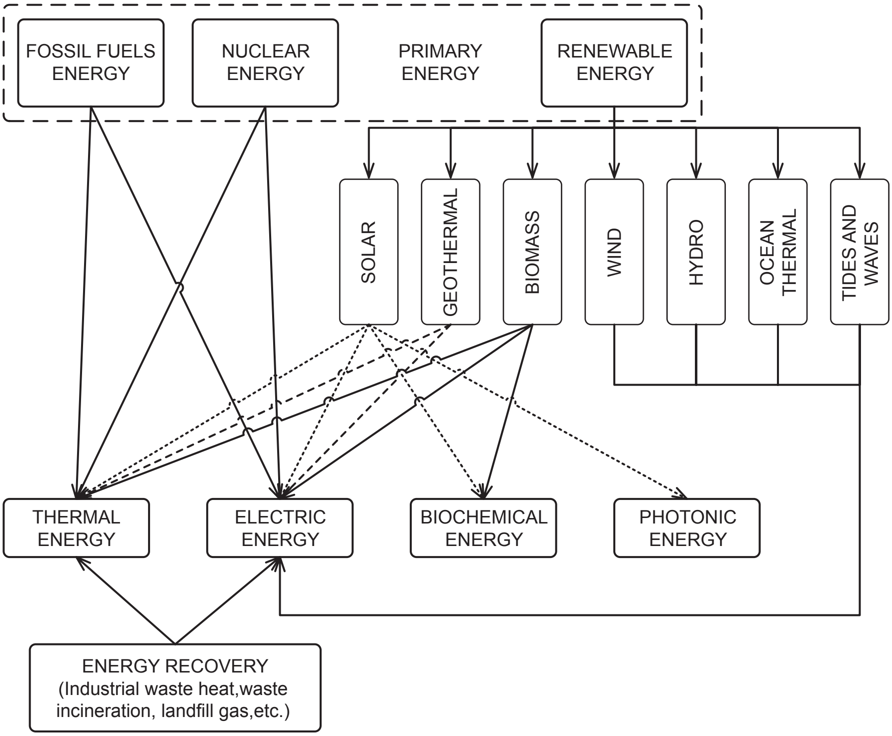

Fig. 5.1 Paths of generation of basic forms of energy from primary energy

inghouse (2001), and the orbiting aerospace plane "Venture Star" by Boeing and Lockheed-Martin (2002) that uses a mixture of cryogenic liquid–solid H_2 for propulsion. The Japanese hydrogen submarine Urashima 600 was equipped with fuel cells and was launched in 2000. A French submarine with hydrogen and fuel cells with installed power of 300 kW each was built in recent years; it stores the hydrogen in FeTi metal hydrides that contain 1.8 t of fuel onboard. The weight of the storage tank is about 160 t.

Hydrogen can be extracted from a large variety of material resources such as water, fossil hydrocarbons, biomass, hydrogen sulfide, and boron hydrides. In order to extract and separate hydrogen from such material resources, one needs energy. The forms of energy that can drive a hydrogen production process can be classified into four categories, namely thermal, electrical, photonic, and biochemical energy. These kinds of energy can be obtained from primary energy (fossil, nuclear, and renewable) or from recovered energy through various paths, as suggested in Fig. 5.1.

The electrical and thermal energy can be derived from fossil fuels, from renewable energies (such as solar, wind, geothermal, tidal, wave, ocean thermal, hydro, biomass), or from nuclear energy, or from recovered energy such as from industrial waste heat, from municipal waste incineration, and landfill gas. The photonic energy is comprised in solar radiation only, and it is, therefore, of renewable kind. The biochemical energy is stored in organic matter (in form of carbohydrates, glucose, and sugars) and can be manipulated by certain microorganisms that can extract hydrogen from various substrates. In Table 5.3, the main hydrogen production methods are described and the material and energy resources specific to each are listed.

The worldwide hydrogen market is currently valued at over $280 billion/year, growing at 10 %/year, rising to between 20 and 40 %/year by 2020 and anticipated to reach several trillion dollars by 2020. Currently, 18 % of hydrogen production globally sources from coal, 30 % from petroleum, 40 % from natural gas, and 12 % from other source from which an important share is represented by water electrolysis. The sales have increased with 5–6 %/annum in recent years with most of H_2 use in fertilizers industry (50 %) and petroleum industry (37 %).

Hydrogen railway transport represents an essential component of hydrogen economy. As shown in Fig. 5.2, the hydrogen railway transport integrates in the natural water cycle, provided that hydrogen is generated from water by using sustainable production methods. For railway transportation, it appears feasible to store hydrogen onboard in its pure form. Steinberg and Scott [60] presented comparisons of fuel and energy consumption of rail locomotives using hydrogen and other modes of propulsion, against a conventional diesel–electric locomotive and other trains.

Hydrogen train of the future will compete with the electrical train provided that the power is generated in a sustainable manner. Electrified trains transfer more than 85 % of the electricity input to the wheels, making it one of the most efficient transportation systems when compared with private automobiles, buses, or airplanes. Disadvantages of electrification include the capital investment to install electrical substations and catenaries, together with a lack of flexibility for locomotives to move into other service areas not covered by electrification. Table 5.4 gives a summary of hydrogen locomotive initiatives.

In the USA, the Department of Energy launched a program by 1992 on fuel cell development and scaled-up applications aiming to demonstrate the hydrogen technology application on transportation vehicles, including hydrogen locomotives. The key environmental goal of the program has been to provide energy savings and air quality [61]. Another goal is to provide a flexible fuel option and energy savings to the transportation sector. In North America, a consortium has been established in 1990s developing a prototype hydrogen fuel cell hybrid switcher locomotive for urban and military-base rail applications [62].

Development of railway hydrogen propulsion technologies in Japan is reviewed by Ikeya [63]. Hydrogen fuel cell trains were examined by Japan's Railway Technical Research Institute (RTRI) starting with 2001. Some successful small-scale tests were reported: a mini-train running with 1 kW fuel cell (2001); a 30-kW mini locomotive has been moved with 30 km/h in 2004.

Table 5.3 General hydrogen production methods

Method	Description	Material resources	Energy supply
Water electrolysis	Water decomposition into oxygen and hydrogen by passing a direct current which drives electrochemical reactions	Water	Electric
High-temperature steam electrolysis	Steam decomposition by using direct current assisted with thermal energy to drive electrochemical reactions to split the water molecule	Steam	Electric+thermal
Photo-electrochemical water splitting	Use electric and photonic energy to electrolyze water and generate H_2 and O_2	Water	Photonic+electric
Photocatalysis	Use photonic energy and catalysts to decompose water molecule	Water	Photonic
Biophotolysis	Use a reversible reducible cofactor and photometabolically active microbes to generate hydrogen from water, viz. photosynthesis	Water	Photonic+biochemical
Anaerobic digestion (anaerobic fermentation)	Use of biological energy manipulated by microbes to extract hydrogen from biodegradable materials in the absence of oxygen	Biomass	Biochemical
Thermolysis	Use of thermal energy decompose water molecule at very high temperature (~2500ºC)	Water	Thermal
Thermochemical water splitting	Thermally driven chemical reactions performed in a loop with the overall result of water splitting	Water	Thermal
Thermocatalytic cracking	Use of thermal energy to break the carbon–hydrogen bonds of hydrocarbons and eventually generate hydrogen	Fossil fuels	Thermal
Gasification	Converting solid carbonaceous materials (fossil or biofuels, wastes, etc.) into carbon monoxide and hydrogen by reacting them with O_2 and/or steam	Water+fossil fuels+biomass	Thermal
Reforming	Reacts carbon-based liquid or gaseous fuels with steam at high temperature to produce carbon dioxide and hydrogen	Water+fossil or biofuels	Thermal

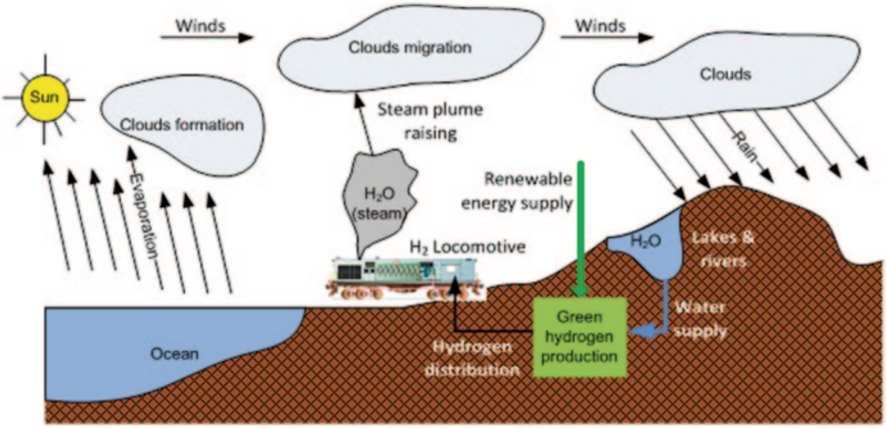

Fig. 5.2 Sustainable hydrogen railway transport integrated with the natural water cycle

In the province of Quebec (Canada), a hydrogen mining locomotive has been demonstrated [64]. In European Union, a project started in 2005 named FELICITAS aiming at development of hydrogen fuel-cell-driven trains capable of meeting the exacting demands of heavy-duty transport for road, rail, and marine applications. The project duration has been of 3 years, and it was a part of the Sixth Framework Programme of the European Research Area. Also in 2005 the Hydrogen Innovation and Research Center (HIRC) of Denmark performed a feasibility study for hydrogen train and its application in Europe.

In Germany, a feasibility study supported by the Environment Ministry of the region Mecklenburg–Vorpommern has been completed and favorably reviewed for the implementation of a hydrogen train in Ruegen (Germany's largest island). The project aims to convert the diesel operated "Arkona Train" to a hydrogen drive.

The Rail Safety and Standards Board (RSSB) of the UK performed a feasibility study of a hydrogen train, including a comparison with other alternative modules. It recommends that Auxiliary Power Units (APUs) are much simpler and less expensive for carrying out train demonstration trials.

Table 5.4 Worldwide hydrogen locomotive initiatives

Country or region	Year(s)	Description and reference or webpage
USA	1992	DoE launches fuel cell program for transportation including hydrogen locomotive [61]
North America	1990s	Consortium establishment for developing a prototype hydrogen fuel cell hybrid switcher locomotive for urban and military-base rail applications [62]
Japan	2001	Japan's Railway Technical Research Institute starts a hydrogen locomotive program of research; proves 1 kW (2001) and 30 kW (2003) mini locomotives [63]; Web page: http://www.greencarcongress.comi
Quebec	2002	Hydrogen mining locomotive in Val d'Or, Quebec [64]
European Union	2005	Project "FELICITAS" extended for 3 years and aiming at development of hydrogen fuel-cell-driven trains for road, rail, and marine applications. Web page http://www.felicitas-fuel-cells.info
Denmark	2005	Hydrogen Innovation and Research Center (HIRC) performed a feasibility study of hydrogen train. Web page: http://www.hydrogentrain.eu
Taiwan	2007	The Taiwan Fuel Cell Partnership has been demonstrated a mini hydrogen locomotive. Web page: http://english.peopledaily.com.cn/200704/13/eng20070413_366270.html
Germany	2008	Project "ARKONA TRAIN" sponsored by Environment Ministry of the region Mecklenburg–Vorpommern aims at conversion of a diesel operated train to hydrogen. Web page: http://www.dwv-info.de/e/news/mirror/wss/wse996.htm#Ruegeni
UK	2008	Feasibility study of the Rail Safety and Standards Board (RSSB) recommending that Auxiliary Power Units (APUs) for carrying out train demonstration trials. Web page: http://www.rssb.co.uki
Ontario	2008	Several studies at University of Ontario Institute of Technology were sponsored by Ontario Research Excellence Fund, Atomic Energy of Canada Limited, and Natural Sciences and Engineering Research Council of Canada for hydrogen locomotive application in Greater Toronto Area [65–68]
USA	2009	Burlington Northern Santa Fe (BNSF) railway company unveiled its first hydrail switch locomotive, powered by hydrogen fuel cells. Web page: http://www.greencarcongress.com/2009/06/bnsf-20090630.html
China	2010	Light-rail hydrogen locomotive with proton exchange membrane fuel cell [69]

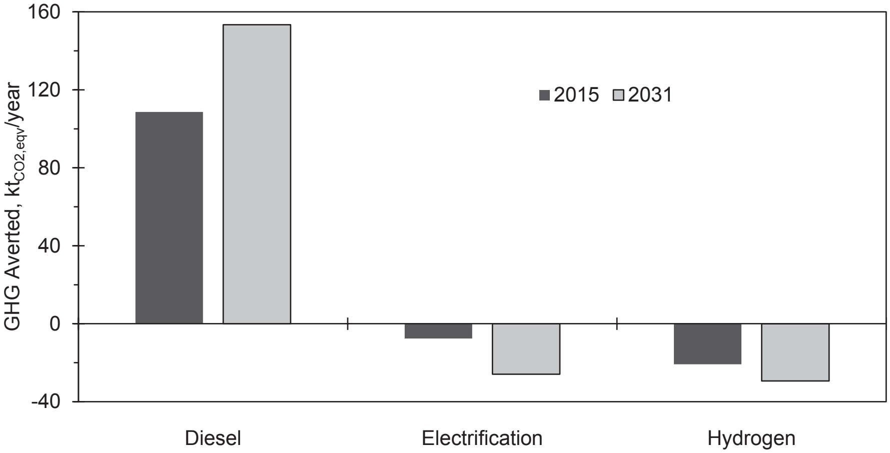

Fig. 5.3 Total equivalent GHGs averted by train transport. (Data from [66])

A comprehensive feasibility study and analysis of hydrogen fuel cell locomotive for Greater Toronto Area (GTA) in Ontario has been pursued at University of Ontario Institute of Technology [65–68]. In GTA, there is a so-called GO Transit Lakeshore corridor, through Toronto, between Oshawa and Hamilton, Ontario, which currently carries a total of approximately 100,000 passengers each weekday. As mentioned in other places within this book, the Lakeshore corridor operates locomotives on diesel fuel at a rate of approximately 5 L/km pulling/pushing 10 or 12 carriages with up to 1540 passengers during peak hours. Passenger-use projections for this corridor are expected to grow by about 90 % for Lakeshore East and 65 % for Lakeshore West between 2007 and 2031, respectively. A sensitivity analysis was performed over a range of operational costs for a hydrogen train, with variability of feedstock prices, fuel cell power density, and expected return on capital investment.

According to general estimates [66], the initial capital cost for train electrification in 2007 was in the order of 5.9 billion Canadian dollars. The operation of the electrified corridor varied between 78 and 145 $/train-km, projected to 2015, while hydrogen operation had a cost varying between 79 and 151 $/train-km, with a capital cost varying from 12.5 to 16 %, respectively. According to the estimations from [66], the prime mover is on the order of 0.09 GJ/km, resulting in the prediction of fuel efficiency between 53 and 58 %. One drawback of fuel cell trains is the required refurbishing at approximately 5000 h of operation; much less when compared to a diesel engine that requires a complete overhaul every 15,000–25,000 h of operation, although continual advances are being made to improve fuel cell durability.

Figure 5.3 provides a comparison of averted emissions based on different power sources, against distance travelled by trains annually. On the basis of the source energy, whether nuclear, OPG (Ontario Power Generation) mix in Ontario, Canada, or hydrogen from SMR (steam methane reforming), the utilization of heat rejected from thermal power plants, combined with hydrogen generated through a thermochemical Cu-Cl cycle and PEMFC (proton exchange membrane fuel cell) trains,

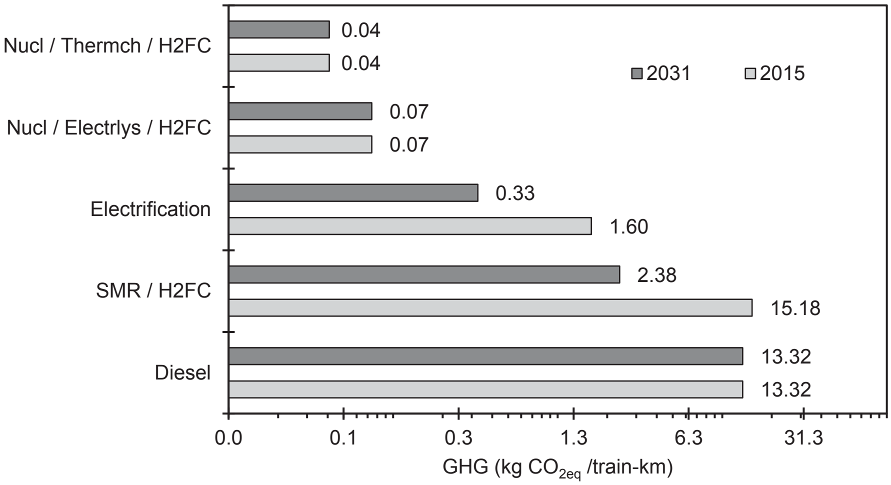

Fig. 5.4 Total GHG emissions from GO trains predicted to 2015 and 2031. (Data from [66])

results in the lowest level of GHG emissions, on the order of 0.10 kg/GJ. The higher efficiency of the PEMFC complements the performance of thermochemical hydrogen production, yielding the lowest GHG emissions at the prime mover, on the order of 0.04 kg/km (345 t by 2015, and 488 t by 2031). The actual impact of CO_2 emission reduction is significant when compared to the diesel alternative. Further GHG emissions forecasts from GO trains—depending on the propulsion option—are indicated in Fig. 5.4.

When comparing the electrification to hydrogen train alternatives, it is assumed that capital expenditures for infrastructure not related to hydrogen remain unchanged. The cost per kilogram of hydrogen is the combined result of several factors, including the capital cost of building the hydrogen plant, the cost of operating and maintaining the plant, the cost of feedstock (whether it is gas, electricity, or thermal energy), the cost of capital invested, the cost of compression and storage, the cost of transportation and delivery, and other miscellaneous external costs not listed here, all included in this analysis.

In the case of electrification, it is necessary to transport the electricity from remote power plants, which may involve up to 9 % transmission losses. These losses are seen as a proportional increase in electricity price (as delivered to the locomotive). Pipeline transportation of hydrogen at high volumes can be as low as $0.1/kg, while liquid hydrogen transportation reaches $0.3/kg. From an economics perspective, the investment required to provide power substations and catenaries for electrification is contrasted with the investment in refueling stations and hydrogen delivery via piping, respectively. Electrical transformer substations in the case of electrification have a cost impact that can be compared to filling stations in the case of hydrogen fuel.

Based on the above results, it appears that the GO hydrogen train is promising with major environmental advantages, but also drawbacks such as high cost and relatively short lifetime of PEMFCs. Scaled-up fuel cells can fit within the existing Bombardier ALP-46 A locomotives, including hydrogen gas storage. The electrification of train operations in the Lakeshore corridor may also be affected by CO_2 legislation in direct proportion to the electricity mix established by Ontario Power Generation. Since this energy mix is projected to contain a portion based on fossil fuels, there is some uncertainty in the potential increase in the cost of operation per train-km. This uncertainty contrasts with the uncertainty of fuel cell prices in the future. While the cost associated with GHG emissions will inevitably increase in the future, the cost of fuel cells is projected to be lower as the technology develops, matures, and reaches mass production.

5.3 Methanol Locomotive Initiatives

An alternative to hydrogen economy has been proposed by George Olah, termed as methanol economy [70]. This is a scenario of sustainable world development in which hydrogen is combined with captured carbon dioxide to generate methanol and dimethyl ether. Commercial technology is already mature for methanol and dimethyl ether synthesis, whereas for carbon dioxide capture from the atmosphere, the technology is under development.

Carbon dioxide can be alternatively captured from combustion processes where it is densely emitted; known technologies can be applied in this respect such as those based on CO_2 absorption. Methanol can be used as a near direct substitute for gasoline, or it can be used as fuel in direct methanol fuel cells. Dimethyl ether (DME), a compound easily created from methanol, can be used as a near direct substituted for propane and has also been shown to be a promising substitute for diesel fuel with only minor engine modifications. Because methanol has a normal boiling point at 65 °C and freezing point at −97 °C and is chemically compatible with gasoline, there is practically no need to create a new infrastructure for methanol as a fuel. In addition, the DME can be benefited by propane infrastructure, already in place.

In order to be sustainable, the methanol economy must integrate within two natural cycles: water cycle and carbon dioxide cycle. Figure 5.5 shows the layout of a sustainable railway transportation based on the methanol economy. The weak link for the implementation of a global methanol economy is the nonexistence of a large-scale commercial technology for carbon dioxide capture from the atmosphere, although this process is demonstrated by laboratory prototypes.

Some methanol economy initiatives including its railway application are given in Table 5.6. There has been much enthusiasm on alcoholic fuels in 1980s when the research had been motivated by various fuel crises. The baseline is the research performed in the USA by the Southwest Research Institute which published extensively on this subject, as summarized in [71]. Further research on these technologies has been pursued in South Africa and Brazil which had major economic interest on promoting biofuels. Methanol locomotives were tested by the Energy Company of Sao Paolo and South African Transport Services [72].

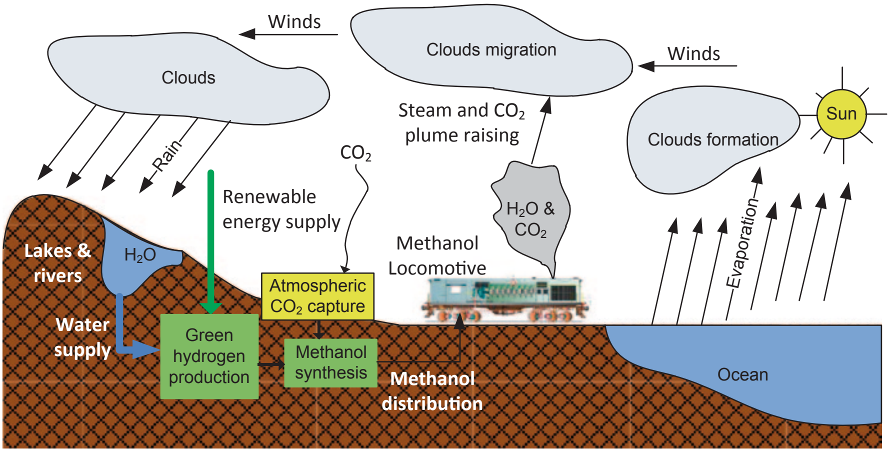

Fig. 5.5 Sustainable methanol railway transport, integrated with the water and carbon dioxide natural cycles

Table 5.6 Methanol fuel initiatives with focus on railway transportation

Country or region	Year(s)	Description and reference or webpage
USA	1980	Southwest Research Institute initiated a direct injected two-stroke locomotive engine development program. The locomotive can operate as dual diesel–methanol fuel [71]
Brazil	1981	CESP—Energy Company of Sao Paolo, initiated a research and development program and started tests on a methanol railway locomotive [72]
South Africa	1983	A consortium formed by South African Universities, Sasol Alcohls, South African Department agriculture and Fisheries, South African Transport Services started implementing a program toward oxygenated fuels for transportation by expanding their methanol/ethanol/propanol production. It investigates the possibilities of using alcohols to railway systems by converting to spark ignition engines [72]
USA	1989	Methanol Institute is founded as a non-profit organization with the purpose to lobby the US Congress to support methanol fuel markets. Web page: http://www.methanol.org/
Canada	2008	Blue Fuel Energy—a Canadian company in British Columbia—started to implement green methanol production from biomass. Web page: http://bluefuelenergy.com/

5.4 Ammonia Locomotive Initiatives

Another alternative to hydrogen economy is known as the ammonia economy introduced by MacKenzie, Avery in 1986 [73] . In this energy pathway, hydrogen is not used directly. Rather, hydrogen is produced from water and then combined with nitrogen extracted from air. Ammonia is then used as transportation fuel for vehicles where it can be combusted while expelling steam and nitrogen back to the

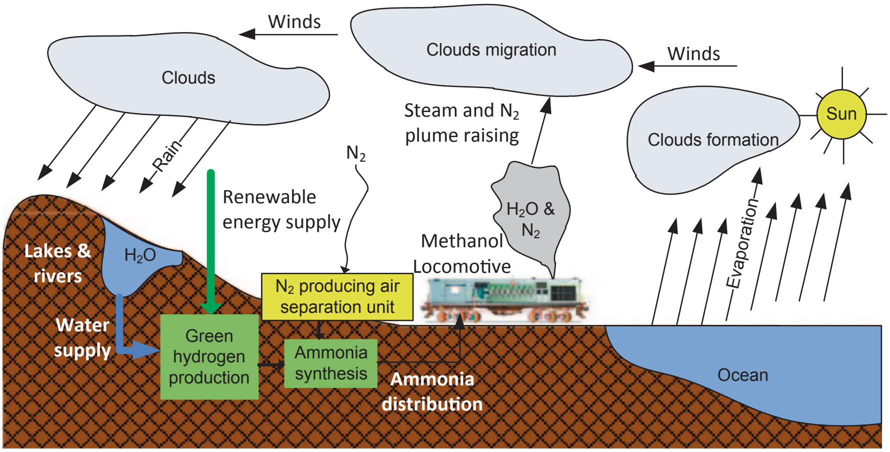

Fig. 5.6 Sustainable ammonia railway transport, integrated with the water and nitrogen natural cycles

atmosphere. A sustainable ammonia economy must be integrated with water and nitrogen cycle in nature. Figure 5.6 shows the layout of ammonia-based railway transportation. Large-scale air separation units are used to extract nitrogen from the atmosphere. This technology is already mature and available. Hydrogen can be extracted from water using large-scale electrolysis plants driven with power derived from nuclear, hydro, or wind energy or other renewable sources. Once hydrogen and nitrogen are extracted from air and water, ammonia can be synthesized based of the well-established Haber–Bosch process. While used on a transportation vehicle, ammonia produces propulsion power while transforming itself into steam and nitrogen which are released back into the environment.

Commercial plants using the Haber–Bosch process produce millions of tonnes per year of ammonia for the fertilizer industry. There is already an infrastructure in place for handling ammonia given its current widespread use as a fertilizer. Pipelines throughout the American Midwest and other countries already transport liquefied ammonia in a similar manner to natural gas. There is a considerable experience of distributing ammonia with trucks, barges, ships, and rail. In road transport, the typical cisterns have 45 kL capacity, while rail cars have ~ 130 L. Ocean ships transport ammonia in low-temperature storage tanks in capacities up to 50 kt. It is estimated that an “Ammonia Economy” would be considerable cheaper than hydrogen to implement from both transportation.

The downside of the ammonia technology resides from the lack of development of ammonia engines and direct ammonia fuel cells. Although not being mature, these are proven technology. Another aspect—which is shared with any version of hydrogen economy—is the lack of large-scale hydrogen production technology from renewables and nuclear. There is, however, a major advantage of ammonia economy when compared with methanol and hydrogen economies discussed above: This is the ability of ammonia to be stored seasonally. Because of the major inter-

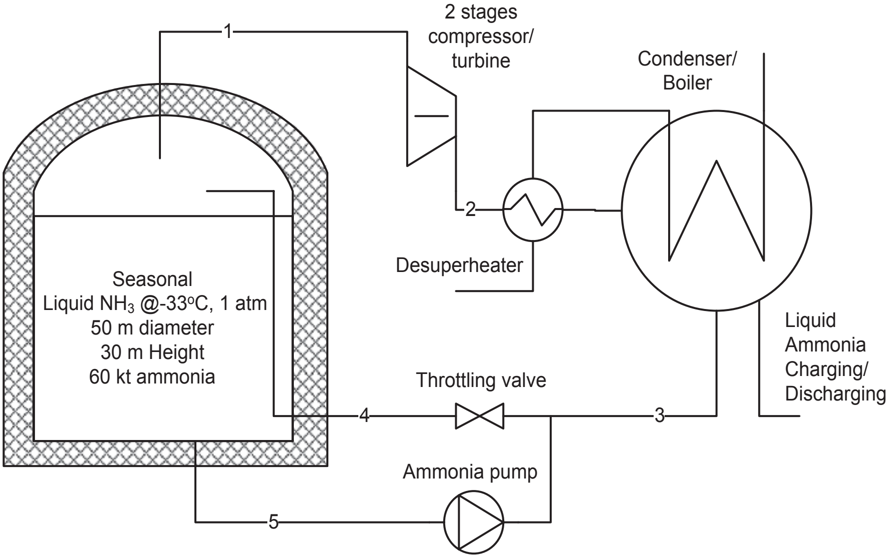

Fig. 5.7 Seasonal large-scale refrigerated ammonia storage system

est in industrial ammonia as a fertilizer, large-capacity seasonal storage tanks were developed. Ammonia demand peaks during the summer when it must be spread on agricultural fields. Ammonia is produced throughout the year, and the winter production is stored for the summer season.

Tanks with a capacity of 15,000–60,000 m^3 were constructed before the 1970s. Ammonia is stored in refrigerated state at ambient pressure and its normal boiling point, which is −33 °C. The tanks of cylindrical construction of 38–52 m inner diameter and 18–32 m useful heights were built. In order to compensate for the heat penetrations, whole construction is well insulated (double-wall technology is used) and compressors are employed to remove the heat by simulating a refrigeration plant for which the tank plays the role of evaporator. Basically, ammonia vapors existing above the liquid are aspired by compressors and delivered at a high pressure where they are condensed and the liquid is returned back to the tank. In this way, the temperature and the pressure in the tank are kept constant.

Figure 5.7 presents a typical seasonal ammonia storage system. Cold vapors in 1 are aspired and compressed with a two-stage compression station up to state 2 that corresponds to a condensation temperature for winter season. The liquid condensate at ambient temperature in 3 is throttled and returned as a cold two-phase vapor liquid mixture into the tank. The circulated ammonia flow rate must be such that it compensates for the effect of heat penetration from outside and the associated ammonia evaporation. In practice, 0.1 % from stored liquid evaporates per day. The latent heat of ammonia at 1 bar is 1370 kJ/kg; thus, about 1.4 kJ of cooling must be provided per kg of liquid ammonia, each day.

During winter time, ammonia refrigeration plants operating at −33°C evaporation and +15 °C condensation temperature with a condensation can achieve COP=2.5; therefore, the corresponding compressor shaft energy is 0.6 kJ/kg every day, or 110 kJ/kg per 6 months of storage. The total energy for running a 60-kt tank is therefore 6.6 GJ per storage season (season =6 months winter-to-summer storage period). Charging of ammonia into tank is normally by liquid at high pressure, i.e., at condenser level. During charging, the liquid is expanded to 1 bar; therefore, the cooling demand is only the requirement to condense the fraction of generated vapor. Vapor fraction in winter condition during ammonia filling is ~15 %; therefore, about 9 kt vapors must be condensed for the 60 kt tank, or 4.9 GJ shaft energy must be provided for complete filling. In total, the needed shaft energy to drive refrigeration is ~11.5 GJ per season.

Table 5.7 gives the ammonia fuel initiatives with focus to railway transportation. There is history of using ammonia as fuel in transportation vehicles including street cars as described in [77]. First trials of ammonia engine were dated since the last years of the nineteenth century. During the Second World War, ammonia has been used as a replacement fuel for bus transportation. Many research initiatives of using ammonia for road vehicles can be remarked in recent years, as reviewed in [77]. An ammonia locomotive study has been initiated in the USA by a private company in 2006, as given in Table 5.7. The system is based on an indirect ammonia fuel cell. A comprehensive feasibility study on ammonia locomotive and railway shifting to ammonia was pursued in Canada, at University of Ontario Institute of Technology. It is shown that ammonia as a transportation fuel offers a carbon-free, hydrogen-rich energy resource that emits no greenhouse gases on complete combustion and has no global warming potential. Furthermore, it may be produced from any renewable energy resource and is a strong option for long-term sustainability. Ammonia also provides a pathway toward a hydrogen economy, which is widely considered as the ideal for long-term environmental sustainability.

In total, ten configurations are investigated for ammonia locomotive at UOIT [34], including the diesel-fueled locomotive baseline, and the performance gains are considered against economic factors for fuel and equipment costs in a comparative assessment. From the modeled results for the systems with 50-% fuel energy input replaced by ammonia, and partial decomposition to produce hydrogen fuel using engine waste heat to assist combustion, diesel fuel consumption, is reduced from 0.21 kg/s to less than 0.10 kg/s, with an associated reduction in GHG emissions of over 8 t-CO_{2eq} per day for a typical locomotive duty cycle. Criteria air contaminant emissions of NOx and HC are reduced below emissions levels outlined for the upcoming Tier 3 requirements, while PM emissions meet current Tier 2 requirements.

5.5 North American Natural Gas Locomotive Initiatives

Locomotives fueled with natural gas represent an interesting and feasible transition alternative toward cleaner emissions. Indeed, natural gas emissions are less GHG polluting than current diesel-fueled emission for locomotives. There are two pos-

Table 5.7 Ammonia fuel initiatives with focus on railway transportation

Country	Year(s)	Description and reference or webpage
Canada	1981	Hydrofuel company based in Toronto converts a 1981 Chevy Imapla to run on ammonia only with a small amount of combustion enhancing additive (acetylene) [74]
USA	2003	Hydrogen energy center—a private company located in Iowa started manufacturing ammonia internal combustion engine based on a Ford 4900 cc 6-cylinder with dual fuel ammonia–propane, and single fuel ammonia with boosting from hydrogen generated onboard by ammonia decomposition [75]
USA	2004	The Iowa energy center started to promote ammonia as a transportation fuel by various programs and an annual conference. It assisted the founding of the Ammonia Fuel Association. Web page: http://nh3fuelassociation.org/ Ammonia Fuel Conference is launched: http://nh3fuelassociation.org/events-conferences/
USA	2006	Department of transportation conducted a study on ammonia as vehicle fuel found that is economically meaningful to convert 80 % of the vehicles to ammonia [76]. The private company Vehicle Projects LLC, based on Denver, initiates a project on ammonia fuel for rail transportation, including the development of an ammonia fuel cell. The system works with NH_3 only which is partially decomposed to generate onboard H_2 for combustion boosting. Web page: https://nh3fuel.files.wordpress.com/2012/05/vehicleprojects.pdf
USA	2007	NH_3 Car a private initiative is launched as a start-up company which produced a prototype of ammonia car based on a throttle-body injected 1991 Chevrolet S-10 pickup. The system mixes NH3 and gasoline in the carburetor in 60/40 ratio.
Canada	2008	At University of Ontario Institute of technology, an ammonia–fuel program has been started. This program has been partly founded though the Ontario Partnership for Innovation and Commercialization and by the Federal Economic Development Agency for Southern Ontario. An ammonia membrane catalytic reactor has been prototyped and nine schemes for ammonia use as fuel for transportation developed [77]
USA	2010	National Center for Manufacturing Science (NCMS) in association with Clinton Foundation stared economic initiatives toward ammonia fuel. Web page: http://www.ncms.org/
Canada	2013	Transport Canada funds the University of Ontario Institute of Technology to investigate the feasibility of ammonia train for the Greater Toronto Area. The funding is granted through the Clean Rail Initiative of Transport Canada. Nine concepts of ammonia-based fuel locomotives were proposed [34]

sibilities of storing natural gas for railway transport: compressed natural gas (CNG) or liquefied natural gas (LNG). In the last version, the LNG, almost pure methane is cooled and stored at cryogenic temperature.

There are two established concepts to convert the current two-stroke diesel engines for locomotives to LNG. In a low-pressure approach established in the 1990s by the American company Energy Conversion Inc. [78], natural gas vapors are extracted from the LNG tender car and then heated and injected into the two-stroke engine through a special low-pressure injector which opens at the time immediately after the intake port is closed. The natural gas fuel is compressed together with air, and then, a small pilot injection of diesel fuel is given at the top dead end to ignite. This system has major benefits because it reduces NOx emissions since injecting of less diesel lowers the combustion temperature, it eliminates the need of boil-off methane venting because cryogenic vapor is drawn from the tank for fueling. Although this system is safe and allows for dual operation (diesel-only or LNG-diesel), there is a technical difficulty as the required injection pressure should be higher than 7 bar (absolute). However, during the operation, the pressure in the cistern can be lower or fluctuate and engine remains suddenly without fuel.

Table 5.8 gives some North American initiatives toward the development of natural gas locomotives. The development of natural gas locomotive has been initiated in 1980 by Burlington Northern (BN) railway which first focused on natural gas. They first developed a natural gas engine converted from a diesel locomotive engine known as EMD 567. This engine has been installed and tested in a converted form to a GP9 locomotive. It does not pose any major development problem. However, the volume of the CNG storage tank is considered too large to be accommodated for a normal hauling locomotive ride.

In 1987, BN has partnered with Air Products and Chemicals Inc. and started to develop a LNG-fueled locomotive system. The selected engine for conversion has been the EMD 645 E3B characterized by high power and operation in a turbo-

Table 5.8 Natural gas fuel initiatives for railway locomotives in North America

Country	Year(s)	Description and reference or webpage
USA	1983	Burlingon Northern (BN) railway partnered with Commercial Sales Inc. (Tahoma) to develop a CNG locomotive on an EMD 567 engine, installed on GP 9 locomotive [78]
	1987	Burlingon Northern (BN) associated with Air Products and Chemicals Inc. to develop a LNG locomotive based on a high-horsepower turbocharged EMD 645 EB3 diesel engine to dual fuel. It has been incorporated into BN SD40-2 7890 initiative. This research program concluded after approximately 6 years [78]
Canada	1999	Transport Canada funded a research on natural gas-fueled railway locomotive technology. The study has been completed by “Engine Systems Development Centre” [81]
Canada	2013	An initiative of Canadian National (CN) Railway was fruitfully accomplished by demonstrating an experimental tender pilot project of liquefied natural gas locomotive with dual fueling. The system uses 90 % natural gas in form of LNG combined with 10 % diesel fuel stored in a regular tank. A 480-km trip has demonstrated the project between Edmonton and Fort McMurray in Alberta [82]
Canada	2014	Transport Canada funds the University of Ontario Institute of Technology to investigate the smart energy management option for CNG locomotive system. The funding is granted through the Clean Rail Initiative of Transport, Canada. Six concepts of LNG-based fuel locomotives were proposed [83]

charged mode. The engine has been installed on a BN SD 40−2 7890 locomotive. The engine conversion involved the redesign of the piston and design and fabrication of new fuel injectors. When it operates with LNG, the cooling effect obtained when the fuel is heated up from cryogenic temperature is used to cool down the intake air to reduce the work input required by the compression step of the turbocharger.

The fueling system promoted by Westport and known as HDPI (high-pressure direct injection) [80] injects natural gas in the late compression stroke. An integrated system is proposed by Westport which includes a fumigated low-power engine supplied with the boiled-off LNG which turns a cryogenic pump to pressurize the liquid fuel up to 200 atm for injection. Nevertheless, the major disadvantage of the HDPI engine is that it is not designed for diesel-only operation, and therefore, this system is closely related to the LNG infrastructure development.

In a recent patent [79], Westport Inc. came up with a fueling solution that allows for natural gas supply at controlled pressure from the cryogenic tank. They use a positive displacement pump able to displace a two-phase mixture. The vapor/liquid fraction at pump intake can be adjusted automatically, in function of the needs. Although Westport applied this system for high-pressure injection (200 atm), it can definitely work for low-pressure injection systems as well.

Other possible power plants were discussed in scholarly papers; these involve the use of solid oxide fuel cells for rail locomotives, when the fuel is methane. It is possible to integrate the methane reforming process with the solid oxide fuel cell. A complete diagram of an SOFC system is presented in Fig. 5.8 from [88].

Air from the ambient is aspired by the air compressor in #1 and discharged at high pressure in #2 with further preheating (#2–#3); preheated air is fed in fuel cell in #3. The oxygen-depleted air is discharged at the cathode side in #4. Natural gas enters in 5 and is preheated (#5–#6) and mixed with superheated steam recycled

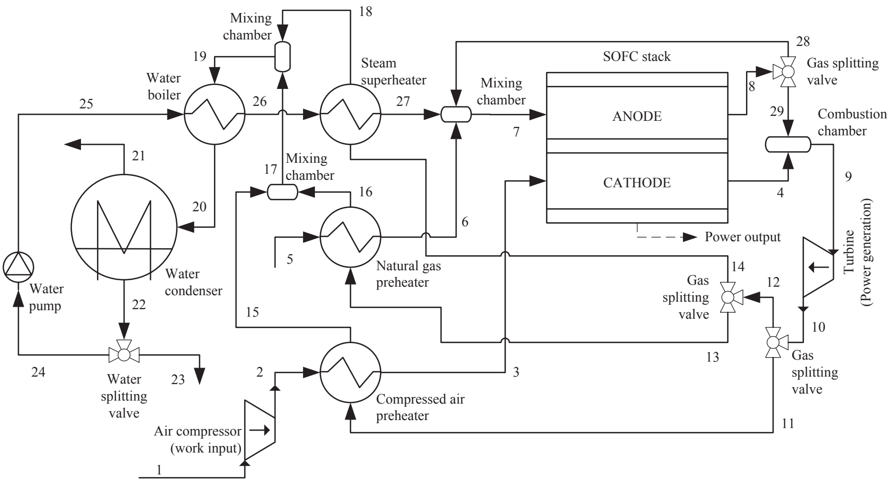

Fig. 5.8 SOFC/gas turbine power generation using natural gas fuel [88]

from the fuel cell stack #28 and extracted from the exhaust gases #27. The makeup gas consisting in natural gas, steam, un-combusted gases (hydrogen, methane, and carbon monoxide) enters at the fuel cell anode in #7. The product gas exhaust at anode #8 is split into two streams—stream #28 (recycled) and stream #29 directed toward the combustion chamber, where it combusts with oxygen-depleted air from the cathode #4, producing hot exhaust gas in #9.

The exhaust gas at high temperature and pressure in #9 is expanded with work generation in the gas turbine and retrieved downstream in #10, where it is split into three streams to be used for heat recovery (steams #11, #13, #14). The enthalpy of these gases is used for preheating air, preheating natural gas, and superheating steam. After this, all three streams are mixed in #19 and their enthalpy used for steam generation from recovered water in the water boiler. Colder exhaust gases in #20 (assumed completely combusted) are further cooled in the water condenser which condensates water while releasing the uncondensable gases in #21. The resulting water is partially drained #23 (or used for other purposes) and partially recycled #24. The recycled water is first pressurized (#24–#25), then boiled (#25–#26) and the resulted steam superheated (#26–#27).

5.6 Other Clean Rail Initiatives

In general, the clean rail initiatives are focused on the opportunity of electric vs. diesel locomotives. Some of the initiatives promote fuel cells as a method for enhances fuel economy. Most of the initiative project concentrates on reducing the emissions such as NOx by applying a selective catalytic reduction system and diesel particulate filters. The application of diesel particulate filter (DPF) has been investigated in two project initiatives at South Coast Air Quality management District [84] and contracted to Miratech Corporation (USA). These involved the application of DPF to switch locomotive (for the first project) and to head end power generators of a line train (the second project). Note that a head end power generator is installed at each passenger railcar to run gen-sets continuously, consuming diesel and producing air pollution. The first project tested the DPF application to an EMD locomotive for expected 90 % reduction in the particulate matter (PM) emissions. The second project demonstrated 90 % reduction in NOx and PM emissions to passenger train gen-sets.

Some other after-treatment projects initiatives are reviewed here based on [85]:

- German freight locomotive retrofits projects with the addition of DPF and SCR in Kiel; locomotives series MaK 1700, 1206, 2000BB; the model 1206 is used in Eurotunnel transport; it uses a scrubber wagon
- Massachusetts Bay Transportation Authority implement oxy-catalysts on EMD F40 locomotives
- UP Railway implements oxy-catalysts on EMD SD60M locomotives

- UP and BNSF project funded by \$5 million, implementing DPF on EMD MP-15DC
- California Air Resource Board (CARB) Emission program encourages a voluntary PM reduction by the railway operators

Biodiesel as a clean fuel for locomotives has been studied within various project initiatives to determine its potential. Transport Canada had a funding initiative finalized with a feasibility study regarding biodiesel for locomotives. It is shown that biodiesel of blended diesel/biodiesel can be used in Canadian locomotives manufactured before the year 2000. Due to EPA regulation issues, the newer locomotives require more stringent emissions compliances and thenceforth have to be tested with respect to fuel blend. More specifically, the durability of the biodiesel is the main unknown to be investigated [86].

In 2000, the National Renewable Energy Laboratory (USA) had the initiative to study the feasibility of biodiesel in locomotive engines. The study has been granted to the Southwest Research Institute at San Antonio (TX) and involved more specifically the implementation of biodiesel on the EMD GP38-2 locomotive [87]. There was field test pursued on that type of locomotive rated at 2 MW full-rated power. It has been demonstrated that the locomotive achieved 98 % of its full-rated power using biodiesel. It has been concluded that long-term durability tests are required.

5.7 Concluding Remarks

In this chapter, some relevant clean rail initiatives are reviewed. It is clear that utilization of diesel fuel and the power generation process required for electrified railways is damaging the atmosphere by the emissions of various polluting gases of which the carbon dioxide is the most abundant. Many jurisdictions and private institutions realized therefore the importance of clean rail initiatives aiming at promoting a clean railway transportation.

The most funded initiatives are in the area of hydrogen energy. As shown, hydrogen energy concept depicts the promise that in the future, the humankind relates to hydrogen as an energy carrier and chemical feedstock. In order to achieve such a scenario, a railway operation must be integrated sustainably in the natural water cycle. This means that hydrogen must be produced at large scale from water using renewable (and maybe nuclear) energy.

The projects toward a hydrogen railway demonstration focus on the development of a hydrogen locomotive, with two major options: internal combustion engine and fuel cell. Although the amount of funding and initiatives in this direction are significant, there is no major progress yet. However, the past projects demonstrated clearly the technical feasibility of the hydrogen locomotive, especially when applied to passenger traffic of the highly urbanized areas such as the Greater Toronto Area characterized by high commuting rates.

A sound alternative to hydrogen railway is the methanol locomotive. This again has been demonstrated technically feasible by the effort of few railway operators in USA, Brazil, South Africa, and Canada. The overall economy for a short-term implementation scale is better for methanol economy than for hydrogen economy because methanol is easier to distribute. Methanol economy must integrate with water and carbon dioxide natural cycles in order to be sustainable, which are difficult because of the lack of carbon dioxide capture technology from the atmosphere.

Some few projects on ammonia locomotive exist, but only at the level of feasibility studies. Ammonia is technically proven as fuel or hydrogen source in various alternatives. In the ammonia economy, the fuel cycle for transportation is integrated with the water and nitrogen natural cycle which is very feasible with nowadays technology. A recently funded initiative by Canadian government showed that ammonia locomotive systems can be built and are feasible in a variety of ways, including internal combustion engines and fuel cells. Ammonia can be used as a standalone fuel source with onboard generation of hydrogen for combustion boosting or through direct ammonia fuel cell systems. Furthermore, diesel–ammonia dual fueling is feasible where diesel can be used in limited quantity to boost ammonia combustion.

There are many initiatives throughout various world jurisdictions toward implementation of clean rail options. These initiatives are in general around biodiesel and after-treatment options. Biodiesel has been highly promoted in North America and Europe. There is, however, a lack of knowledge regarding the durability of the biofuel when used on locomotives. The after-treatment technologies became enforced for rail locomotives nowadays. However, the major focus is on the application of particulate matter filters. Some limited projects involved the application of selective catalytic reducers; this development initiative appears to grow.

Chapter 6
Integrated Locomotive Systems

6.1 Introduction

There are ten system configurations investigated in this study. The designs aim to improve overall performance of the locomotive propulsion systems using process integration and multigeneration to more efficiently utilize the energy supplied by fuel and provide additional valuable outputs, thereby improving the overall system efficiency.

Environmental sustainability and green engineering principles are outlined by [89] as guidelines toward the design approach, including:

- Reducing hazardous material and energy inputs/outputs—i.e., reducing diesel consumption and exhaust emissions.
- Prevention of waste formation instead of (or, as well as) waste treatment—i.e., heat recovery processes in place of large engine cooling systems.
- Processes/systems should maximize mass, energy, and space efficiency—i.e., using ammonia simultaneously as a fuel, coolant, working fluid, H_2 source, and NO_x reducing agent.
- Design should integrate interconnectivity with available material and energy flows in processes/systems—i.e., recovered heat is used as process heat to produce additional valuable outputs such as shaft work, cooling, and/or heating.
- Material and energy should be renewable as opposed to depleting.

The proposed systems are introduced in Table 6.1. System 1 is a typical diesel-electric locomotive unit fueled by ultra low sulfur diesel (ULSD) and is considered as a baseline for locomotive operation and performance assessments. In systems 2 and 3, additional ammonia systems are integrated to supply required process heating for selective catalytic reduction (SCR) of exhaust NO_x emissions, and hydrogen fuel production (in system 3), with heat supplied via waste heat recovery from exhaust gas.

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Table 6.1 Integrated locomotive systems considered

System	Brief descriptions[a,b]
System 1	Baseline diesel locomotive unit Diesel-electric locomotive operation, fueled by ULSD System diagram in Fig. 6.1 (16 components, 23 state points)
System 2	Diesel–ammonia (NH_3) locomotive fueling Additional components: NH_3 storage tank (RES-2), NH_3 fuel pump (P2), expansion (throttle) valve (EXP), exhaust heat recovery heat exchanger (HX-1), and SCR System diagram in Fig. 6.7 (21 components, 31 state points)
System 3	Diesel–NH_3–H_2 (+N_2) locomotive fueling Additional components: RES-2, P2, P8, EXP-1, EXP-2, HX-1, SCR, exhaust recovery heat exchangers (HX-2), decomposition, and separation unit (DSU) System diagram in Fig. 6.8 (25 components, 37 state points)
System 4	Diesel–NH_3–H_2 locomotive fueling with N_2 separation and expansion Additional components: RES-2, P2, P8, EXP-1, EXP-2, HX-1, HX-2, SCR, DSU, and N2 Turbine (T2) System diagram in Fig. 6.9 (26 components, 39 state points)
System 5	Diesel–NH_3–H_2 locomotive fueling with NH_3 and N_2 turbines Additional components: RES-2, P2, P8, EXP-2, HX-1, HX-2, SCR, DSU, T2, NH_3 turbine (T3), and H_2 compressor (C2) System diagram in Fig. 6.10 (27 components, 40 state points)
System 6	Diesel–NH_3–H_2 locomotive fueling with engine coolant heat recovery (indirect engine cooling) and NH_3 expansion Additional components: RES-2, P2, EXP-2, EXP-3, HX-1, HX-2, SCR, DSU, T2, T3, C2, engine coolant (jacket water) heat exchanger (HX-3), and NH_3 turbine (T4) System diagram in Fig. 6.11 (29 components, 42 state points)
System 7	Integrated compressed N_2 gas storage Additional components: RES-2, P2, P8, EXP-2, HX-1, HX-2, SCR, DSU, T2, T3, H_2–NH_3 compressor (C2), Exhaust heat recovery/NH_3 heating (HX-3), and N2 storage tank (RES-7) System diagram in Fig. 6.12 (29 components, 42 state points)
System 8	Diesel–NH_3–H_2 locomotive fueling with combined heat recovery and fan powering (radiator cooling) Additional components: RES-2, P2, EXP-2, EXP-3, HX-1, HX-2, HX-3, SCR, DSU, T2, T3, C2, and NH_3 turbine with fan (T4) System diagram in Fig. 6.13 (29 components, 43 state points)
System 9	Diesel–NH_3–H_2 locomotive fueling with NH_3 cab cooling (CAB-C) COPC = 2.0 Additional components: RES-2, P2, EXP-2, EXP-3, HX-1, HX-2, HX-3, SCR, DSU, T3, C2; CAB-C chilled water tank (CH), CAB-C air-cooling heat exchanger (HX-4) System diagram in Fig. 6.14 (28 components, 42 state points)
System 10	Diesel–NH_3–H_2 locomotive fueling with exhaust heat recovery NH_3-RC Additional components: RES-2, P2, EXP-2, EXP-3, HX-1, HX-2, SCR, DSU, T2, T3,T4, C2; NH_3-RC boiler (HX-4), NH_3-RC condenser (HX-5), NH_3-RC turbine (T5) System diagram in Fig. 6.15 (32 components, 45 state points)

[a] Figure elements (components/connections) shown in grey are not included in component listing

[b] Split flows shown in system diagrams (*i*', *i*") are not included in state point count

Systems 4–10 introduce additional options, which further utilize the onboard ammonia for various heat recovery and power generation applications. The recovery processes reduce the energy requirements from diesel fuel by reducing temperature of hot streams to be cooled by radiators, as well as heat energy lost in the exhaust stream, and by supplementing power requirements with the work produced by ammonia subprocesses.

6.2 System 1: Conventional Diesel Locomotive

The operating characteristics of the locomotive prime mover are given in Table 6.2, including engine and cooling system details. These values are applied to each of the system analyses. The baseline system of a typical diesel-electric locomotive powered by a large two-stroke compression ignition diesel engine supplied with ULSD fuel is shown schematically in Fig. 6.1.

During the process, air entering the system is compressed to higher pressure by a given factor, pr_{TC}, in the turbocharger compressor (C1). The air passes through an aftercooler (HX-ac), increasing the density (and therefore mass) of the stream entering the intake manifold, and then is drawn into the engine cylinders. Following internal combustion and expansion stroke, exhaust gases pass through the turbine (T1) of the turbocharger unit, driving the rotor for C1. The combustion gases are exhausted following expansion.

Table 6.2 Prime mover sizing details and locomotive operating conditions. (Sources: [32, 90, 91])

Engine model (EMD)		16V-710G3
Traction horsepower, THP (hp)		4000
Traction power, $\dot{W}_{TP}$ (kW)		2983
Engine speed, N_{ICE1}(rpm)		900
Displacement volume per cylinder, V_d (L)		11.635
Compression ratio, r		16:1
Number of cylinders, n_{cyl}		16
Fuel tank volume, V_{RES1} (L)		8410
Baseline operating conditions		
Turbocharger pressure boost, p_{TC} (~)		1.25
Cooling water reservoir temperature, T_{RES3} (°C)		49
Engine jacket cooling water outlet temperature T_{12} (°C)		85
Heat removal rate[a]	Water jacket cooling, HRR_{wjc} (kJ/kW$_{TP}$ h)	2377
	Aftercooler, HRR_{ac} (kJ/kW$_{TP}$ h)	908

[a] Based on heat removal rates given by [90] for EMD-710 locomotive (converted from Btu/min·bhp)

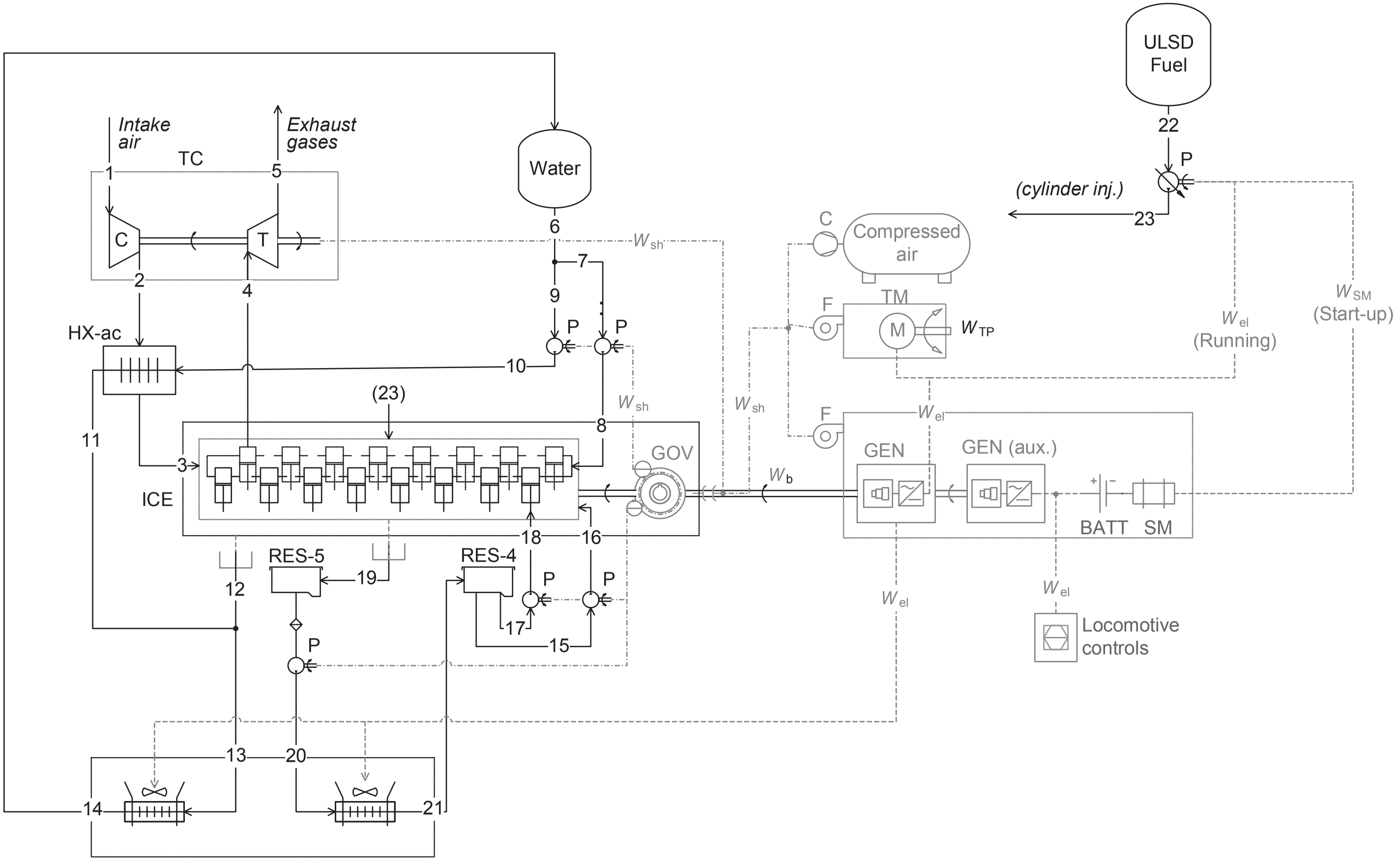


Fig. 6.1 Diesel locomotive system

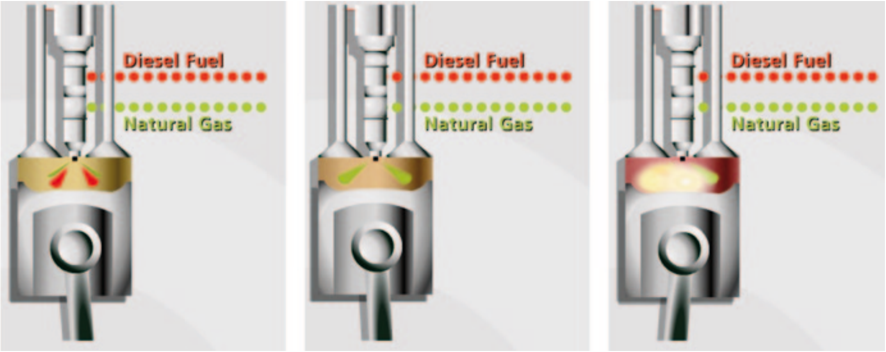


Fig. 6.2 Dual-fuel injection. (Adapted from [92])

6.3 Technology Options for Dual Fueling and Exhaust Treatment

For the possible ammonia-powering options discussed in this chapter, the fuel is either a supply of liquid fuels or a combination of liquid and gas. In the case of liquid-only fueling, NH_3 and diesel fuel may be premixed and injected together into the cylinder; however, for liquid–gas or gas-only mixtures, alternative fuel injection methods must be considered for monofuel direct injection system. For various fuel mixtures, different dual injection systems are suitable depending on the mixture properties. To promote the ignition of secondary fuels, such as the natural gas–diesel injection indicated in Fig. 6.5, a small amount of diesel fuel is piloted into the combustion chamber where it ignites and initiates burning of the secondary fuel injection. This is an attractive option for NH_3 combustion when injected as a liquid fuel, due to the high autoignition temperature, which typically requires high compression ratios to self-ignite in direct injection monofuel engines (Fig. 6.2).

Another arrangement of dual fueling that uses pilot ignition of diesel is high-pressure direct injection (HPDI). Figure 6.3 shows the basic technology, developed by Westport Power, in which diesel fuel is used to ignite high-pressure gaseous fuel, injected at the end of the compression stroke.

Suitable for either liquid or gas fuels, HCCI injection combines the advantages of spark-ignition and compression-ignition engines, by injecting fuel into the cylinder during compression (mixed with air), then using high compression ratio to promote autoignition of the fuel–air mixture. This method allows for higher diesel cycle efficiency levels and lower NO_x emissions, but problems may arise due to unpredictable autoignition conditions in the cylinder, which can cause significant damage to the engine [94].

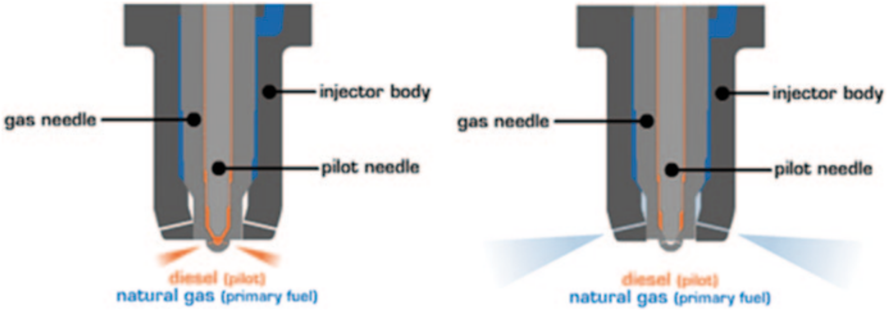
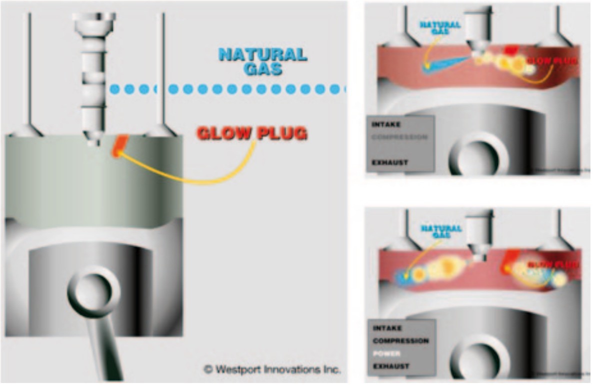


Fig. 6.3 Westport high-pressure direct injection (HPDI) Technology for *natural gas* application. (Adapted from [93])

Fig. 6.4 CNG-direct injection. (Adapted from [95])



For gas-only injection, or for fuels which do not ignite as readily as diesel fuel (such as NH_3 or natural gas), a glow plug can be used to assist ignition instead of the diesel pilot-injection method, as shown in Fig. 6.4, to maintain control of ignition timing. Fuel injected into the cylinder contacts the hot surface of the glow plug, initiating combustion throughout the fuel–air mixture. This is a potential option for injection of partially decomposed ammonia and would not require separation of hydrogen. With sufficient hydrogen production, the need for dual fueling with diesel could potentially be eliminated.

SCR is a widely utilized method of reducing NO_x in combustion exhaust emissions in stationary engines. Ammonia is used as a reducing agent in SCR systems, supplied either directly or in a urea solution, to chemically react with NO_x present in the combustion emissions, producing water vapor and nitrogen gas as products. The reactions and temperature that range through the SCR are given in Table 6.3. The main reaction is dominant for the assumed operating temperature range of 250–450 °C [96] and has a NH_3/NO_x ratio of 1:1, as described by its stoichiometric reaction. At temperatures above 500 °C, NH_3 oxidation occurs causing undesirable NO emissions, and at temperatures below 200 °C the performance of the reaction is too low for NO_x reduction in diesel applications.

Table 6.3 SCR characteristics

Chemical reaction equations	Main	$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$
	Fast	$8NH_3 + 6NO_2 + O_2 \rightarrow 7N_2 + 12H_2O$
	Oxidizing (T > 500 °C)	$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$
Operating temperature range, T_{SCR} (°C)		250–450
Average NO_x reduction for temperature range		0.7–0.9

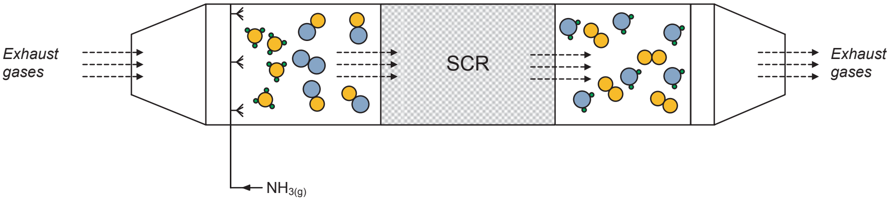


Fig. 6.5 SCR process diagram for main reaction $(4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O)$

The process diagram is shown in Fig. 6.5 for the main reaction. NH_3 vapor is injected into the exhaust upstream of the SCR catalyst. The mixing streams pass through the catalyst bed where the reaction takes place. For the complete reaction, the products leave the catalyst as water vapor and nitrogen gas. Some ammonia slip is possible, which can cause formation of ammonium sulfates and unwanted ammonia in exhaust emissions; the EPA permits an acceptable range of 2–10 ppm ammonia slip [97].

One of the challenges of installing SCR systems in vehicle applications is the large size of SCR units and the vibrations affecting the performance. The Compact SCR™ technology designed by [98] uses shock mounting to damp vibrations and has been installed in an operational 3000-hp 12-cylinder EMD-710G3, a smaller model of the locomotive is considered in the analysis with the same cylinder characteristics. The reported data indicate significant reductions for criteria air contaminants (CAC) emissions (not including SO_x) for line haul and switch locomotive operations, with almost complete elimination of hydrocarbon (HC) emissions. Similar results are reported for commuter locomotives installed with SCR systems in Metrolinx locomotives operating in California [99].

Ammonia is one of the most promising and least expensive methods of storing hydrogen [8]. As a hydrogen carrier, ammonia contains 1.5 mols of hydrogen per mol of ammonia, which amounts to 108 kg H_2/m^3 for liquid ammonia at 20 °C and 8.6 bars [8]. Ammonia can be thermo-catalytically cracked to produce hydrogen using approximately 12 % of the lower heating value of hydrogen [53]. The decomposition occurs according to the endothermic reaction, relative to the hydrogen energy content:

$$\frac{2}{3}NH_3 \rightarrow H_2 + \frac{1}{3}N_2 \qquad \Delta H = 30.1\,\text{kJ/molH}_2 \tag{6.1}$$

Three configurations of ammonia decomposition units that are shown in Fig. 6.6 are tube-type, plate-type, and catalytic membrane. The tube-type (Fig. 6.6a) is the simplest of the options, using a tube filled with the catalytic bed material that is externally heated by passing flue gases. In this type no separation occurs, and all three gas species are present in the product stream. Figure 6.6b shows a plate-type reactor, in which ammonia is fed from the bottom, and flue gas passes through cross-flow channels. Pure hydrogen is separated via selective membrane from the gas stream, and the remainder leaves the reactor as a mixture of nitrogen gas with traces of ammonia and hydrogen. The third type, shown in Fig. 6.6c, separates hydrogen via hydrogen-selective membrane, doped with ammonia cracking catalysts. A nitrogen-selective membrane placed at the outlet gas port is used to improve product separation by shifting the reaction further to the right [8].

There are a variety of catalyst materials that may be used for the decomposition process, but for the temperature range associated with diesel exhaust, ruthenium (Ru) catalysts have favorable performance for NH_3 decomposition for the temperature range considered, operating between 350–525 °C [100, 101]. At temperatures over 1000 K, this reaction occurs without any catalyst; however at lower temperatures, the reaction rate is too slow for the process to be practical for hydrogen production.

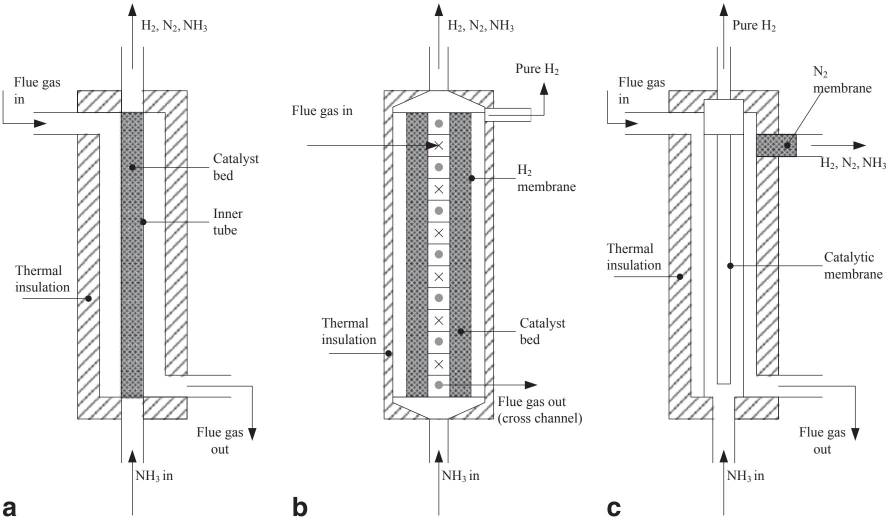


Fig. 6.6 Thermo-catalytic NH_3 DSU options. **a** Tubular catalytic bed reactor. **b** Plate catalytic bed reactor with H_2 membrane. **c** Catalytic membrane reactor. (Adapted from [8])

6.4 System 2: Ammonia Co-Fueling

Ammonia for locomotive fueling and exhaust NO_x emission control is integrated in the system option shown in Fig. 6.7. The ammonia is stored in a pressurized tank at 10 bar (1000 kPa) and is assumed to be a saturated liquid. Fueling is supplied as an NH_3–ULSD liquid mixture, varying the ratio of fuel-energy input between NH_3 and ULSD. Ammonia supply for combustion is pumped from the storage tank and sent with the diesel fuel supply to the cylinder injectors. If a dual-injection system is considered, allowing liquid–gas injection, preheating of the liquid NH_3 fuel may also be included to increase the heat recovery from the exhaust gases and reduce the energy consumed to evaporate and heat the liquid fuel droplets (spray) in the internal combustion engine (ICE) cylinders.

Exhaust NO_x emissions are controlled using SCR. The flow rate of NH_3 required for the SCR process is determined based on the NO_x emission factor for diesel fuel at 1:1 ratio with NO on a molar basis. The liquid is drawn from the ammonia tank and then throttled to atmospheric pressure in the expansion valve. The resulting liquid–vapor mixture enters the exhaust recovery heat exchanger (HX-1) to be heated to a temperature within the considered range of 250–450 °C.

6.5 System 3: Ammonia Co-Fueling with Onboard Hydrogen Production (Without N_2 Separation)

Onboard hydrogen production from ammonia is introduced in the integrated locomotive system shown in Fig. 6.8, based on the concepts described by Dincer and Zamfirescu in [77] for systems-integration approach to use exhaust and other waste heat sources to thermally crack ammonia into hydrogen and nitrogen gases, as described in the background section.

The system is fueled initially with selected ratio for the NH_3–ULSD mixture. A part of the NH_3 supply is pumped to heat exchanger HX-1, where it is heated by the ICE exhaust gases leaving the turbocharger (T1). The ammonia leaves as a superheated vapor and is throttled to a lower pressure. The temperature is reduced by the process; therefore, the NH_3 requires reheating before it can be sent to the DSU.

A portion of the exhaust stream leaving the engine (ICE) is diverted from the turbocharger and is used to reheat the NH_3 to the required decomposition reactor temperature range (400–600 °C). The high temperature NH_3 vapor is split, and the required supply rate for NO_x reduction is directed to the SCR. The temperature in this case is important to consider; if the temperature of the NH_3 stream is higher than 450 °C, it should be cooled before entering the SCR to prevent the formation of undesirable exhaust products.

The remaining high temperature NH_3 vapor enters the decomposition reactor (DSU) where it is thermo-catalytically cracked into NH_3, H_2, and N_2 gases. It is not necessary to separate the streams in this option; the gas mixture is fed directly with diesel fuel into the ICE. The exhaust gas stream that leaves HX-2 is reduced in pressure and mixed with the main exhaust gases before passing through the SCR.

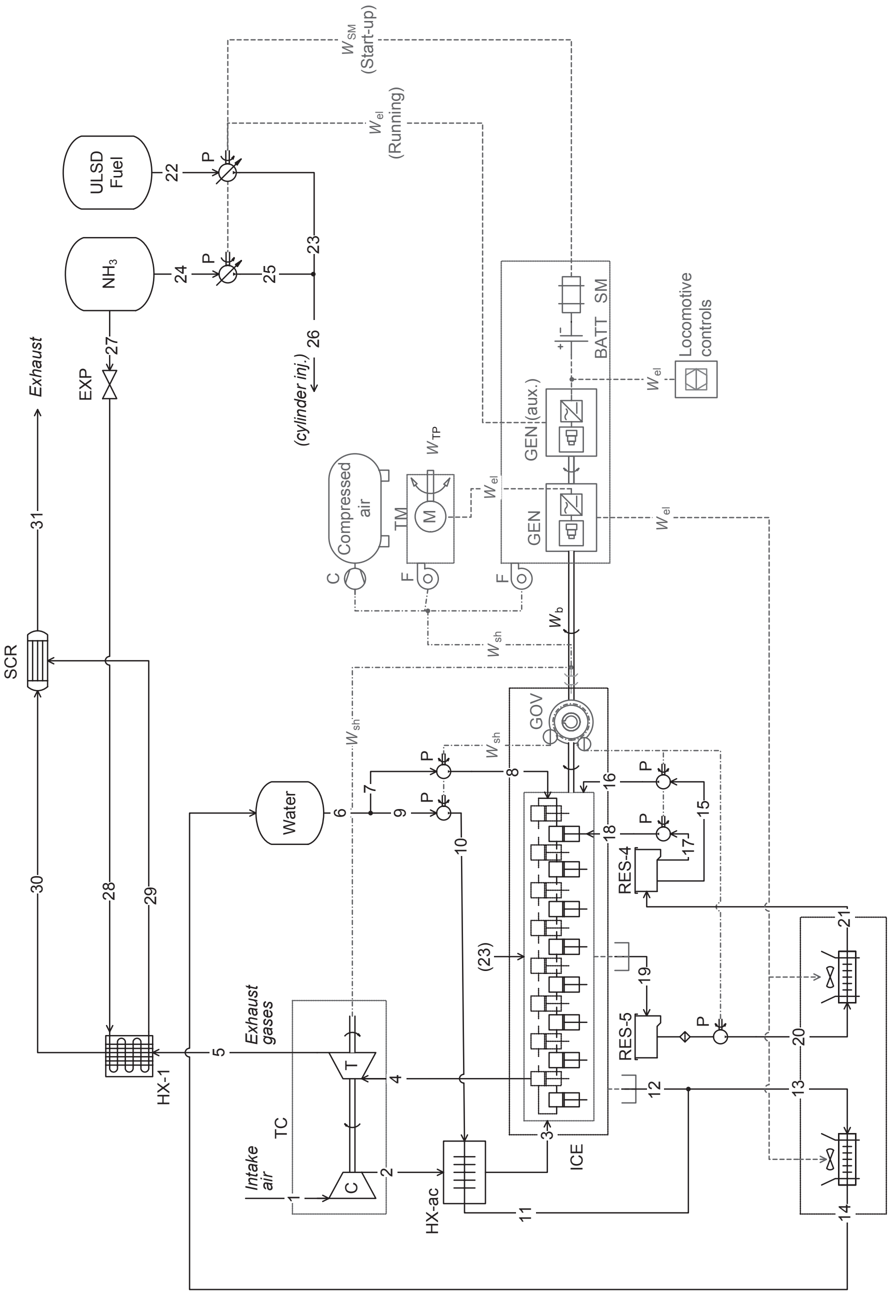


Fig. 6.7 Ammonia co-fueling option

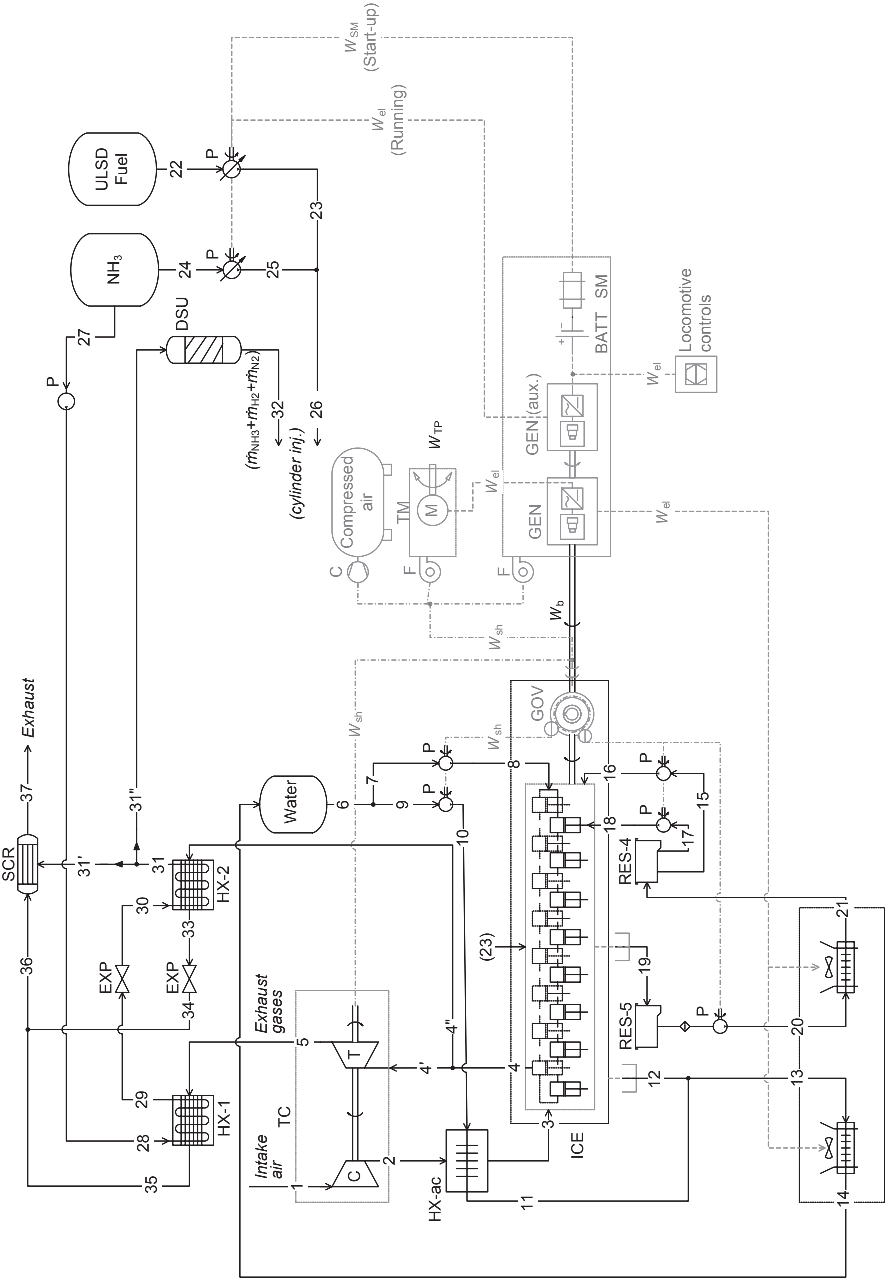


Fig. 6.8 Ammonia co-fueling with onboard hydrogen production (without N_2 Separation)

6.6 System 4: Ammonia Co-Fueling with Onboard Hydrogen Production (with N_2 Separation)

In the fourth approach, exhaust heat is used to thermally crack ammonia into hydrogen and nitrogen gases as described in the previous system option; however, as indicated in Fig. 6.9, the nitrogen gas produced in the reaction is separated and expanded in a turbine, producing shaft work to supplement engine power demands.

Liquid ammonia is pumped through a heat exchanger (HX-1) to recover heat from the turbocharger exhaust and then throttled to a lower pressure. The temperature of the reduced pressure NH_3 stream is raised to the DSU operating temperature range by the ICE exhaust stream through heat exchanger HX-2, leaving as a superheated vapor. A fraction of the NH_3 vapor is supplied to the SCR prior to decomposition for NO_x reduction of exhaust gases. N_2 product gases are sent through the turbine T2 to provide useful work before being exhausted.

The additional work produced by the N_2 turbine is evaluated in the Analysis and Results sections of Chapters 7 and 8… in terms of the change in enthalpy of the gas stream and the isentropic efficiency of the turbine. The NH_3–H_2 gas mixture is fed with ULSD into the locomotive ICE. To fuel with gas and liquid fuels, the approach can be taken to inject the gas stream into the cylinder during compression or to inject with the fuel blend using specialized injectors such as the dual injection systems described earlier.

6.7 System 5: Multistage Heat Recovery with Power Generation

The fifth system, shown in Fig. 6.10, operates in a similar manner to the system described in Sect. 6.6, but it introduces multistage expansion with reheat to increase the overall heat recovery effects by ammonia for the locomotive system. Liquid ammonia is pumped through the heat exchanger HX-1 where it is superheated and subsequently expanded in turbine T3. The gas is reheated in HX-2, and the required supply of NH_3 is directed to the SCR to reduce the NO_x emissions in the exhaust, with the remaining stream passing through the decomposition unit. The N_2 product gas mixture is expanded in turbine T2 and then exhausted to the surroundings. The NH_3–H_2 gas is compressed in C2 and sent with the ULSD stream for ICE injection.

6.8 System 6: Integrated Engine Cooling

The refrigeration effect of ammonia is used to indirectly cool the engine by removing heat from the cooling water as it leaves the engine. As shown in Fig. 6.11, liquid ammonia is drawn from the tank and throttled in an expansion valve to a lower pressure and temperature. The result is a low-temperature liquid–vapor mixture that

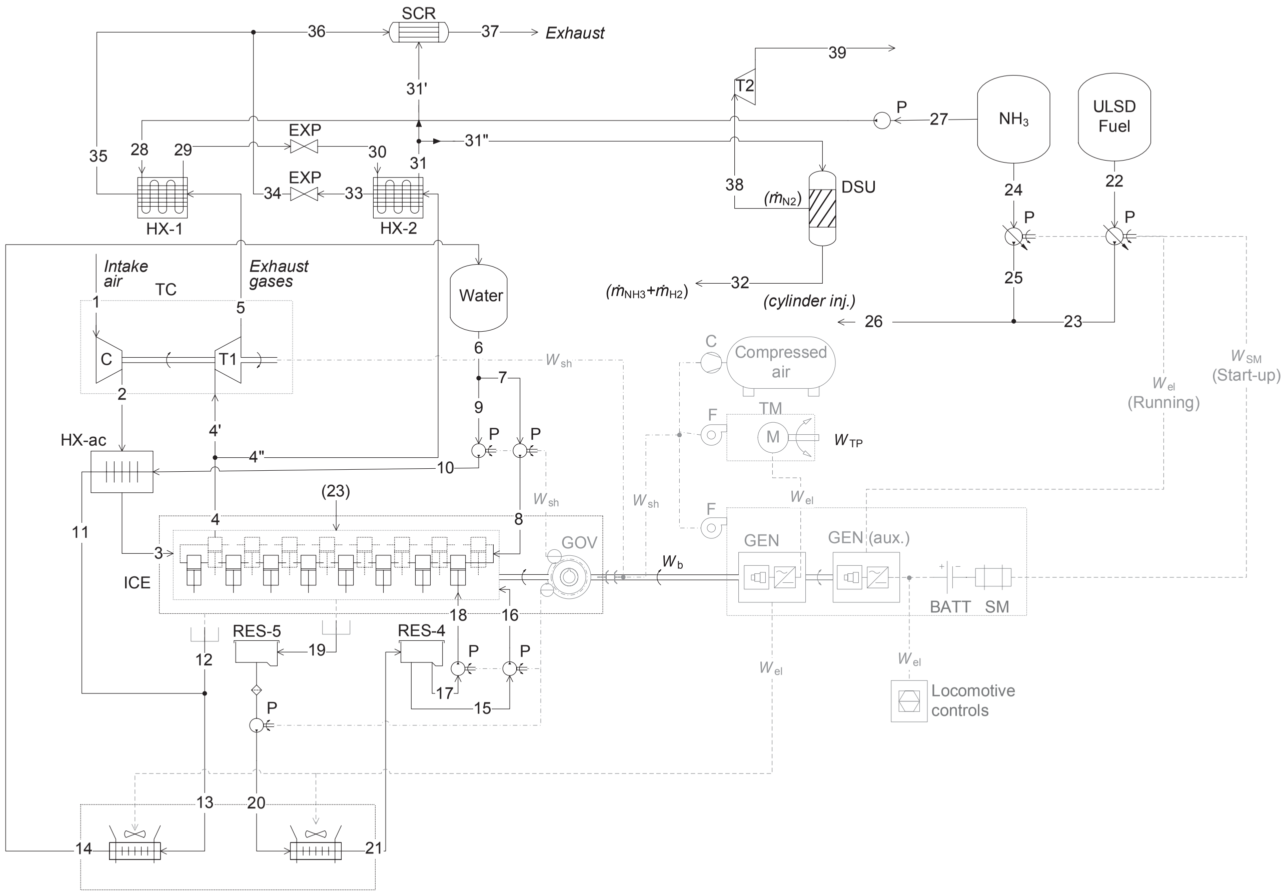


Fig. 6.9 Ammonia co-fueling with onboard hydrogen production (with N_2 Separation)

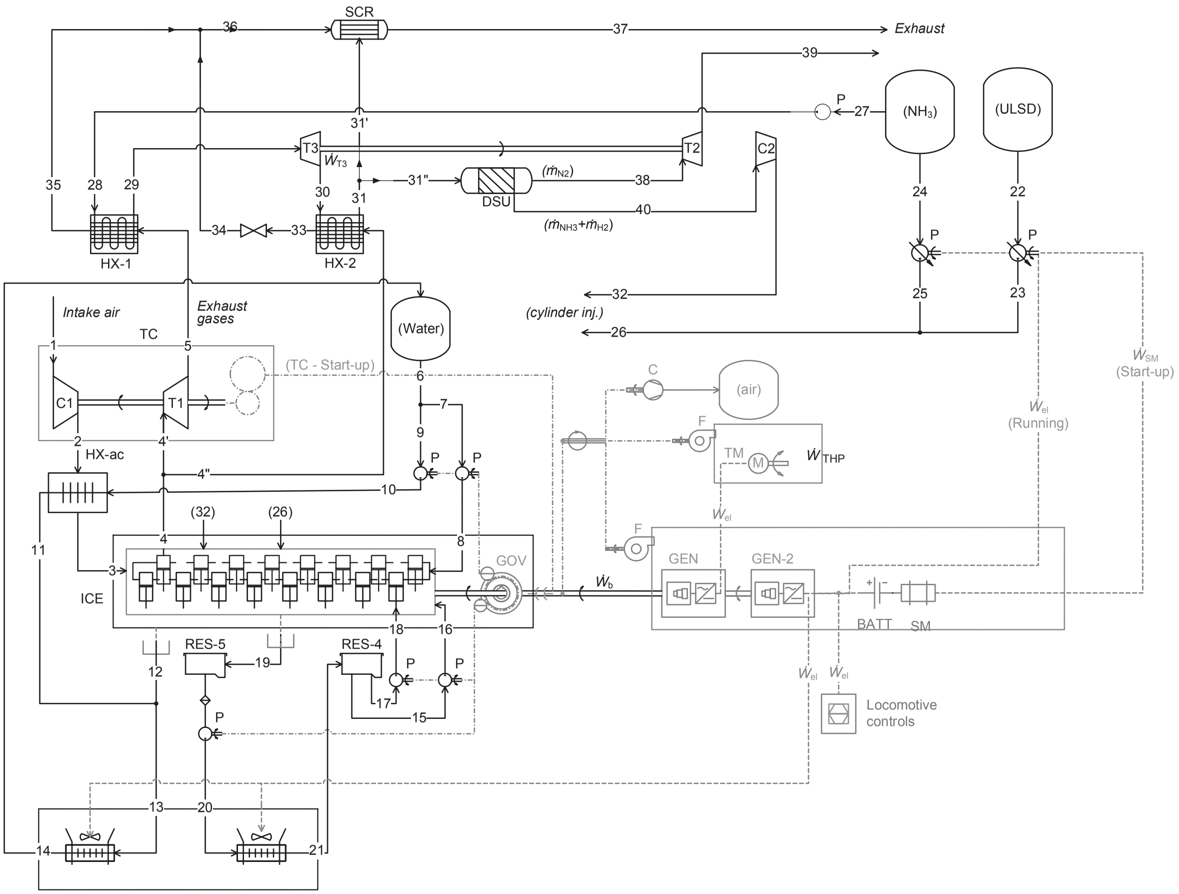


Fig. 6.10 Multistage heat recovery with power generation

can remove heat from the engine cooling water both by latent effect (by evaporation) and sensibly as it passes through HX-3. The resulting vapor is expanded in turbine T4, then passes through the turbocharger exhaust heat exchanger HX-1 for superheating, and expanded again in turbine T3. The stream is then reheated in the high-temperature ICE-exhaust heat exchanger HX-2 at the decomposition reactor operating temperature.

The required flow rate of NH_3 vapor is diverted to the SCR to reduce NO_x emissions, and the remaining NH_3 stream is partially decomposed in the DSU. N_2 is expanded in T2 and then exhausted. The NH_3–H_2 gas is compressed in C2 and injected into the ICE with the ULSD.

6.9 System 7: Integrated Compressed Nitrogen Gas Storage

In the configuration shown in Fig. 6.12, the nitrogen gas exiting the DSU is compressed and stored for production of expansion work on demand. In the DSU, NH_3 is drawn from the tank as a saturated liquid. The NH_3 passes through the heat exchanger HX-3 where it is evaporated before expansion in turbine T2. The stream is superheated in HX-1 and then expanded again in turbine T3.

The stream is reheated in ICE exhaust heat exchanger (HX-2) and the resulting vapor is split into two streams. A small portion of the gas is diverted to the SCR (which is monitored such that the temperature at entry is less than 450 °C), and the majority of the vapor stream is then sent through the DSU for partial decomposition. The N_2 gas is separated from the gas stream, compressed in C4, and then stored in a cylinder in order to supply expansion work on demand. The NH_3–H_2 stream is compressed prior to being sent to the ICE as a gaseous fuel to be combusted with the diesel fuel.

6.10 System 8: Indirect Engine Cooling

Additional engine cooling is integrated in the system configuration shown in Fig. 6.13. The operation is similar to the system 6, with the addition of a cooling fan powered by an ammonia turbine (T4) to increase the indirect cooling effect for the engine. Ammonia is drawn from the tank, throttled to an intermediate pressure, and then directed to HX-3 where it provides some cooling for the engine coolant (water). The ammonia exits as a superheated vapor and is expanded in a turbine (T4) coupled with a rotor to a fan. The fan assists the radiator cooling system, but could be placed wherever needed. Following expansion in T4, the ammonia stream is re-superheated in HX-1 and expanded in T3 to produce shaft work. The low-pressure stream is again re-superheated (HX-2) and the stream is split into the SCR and DSU

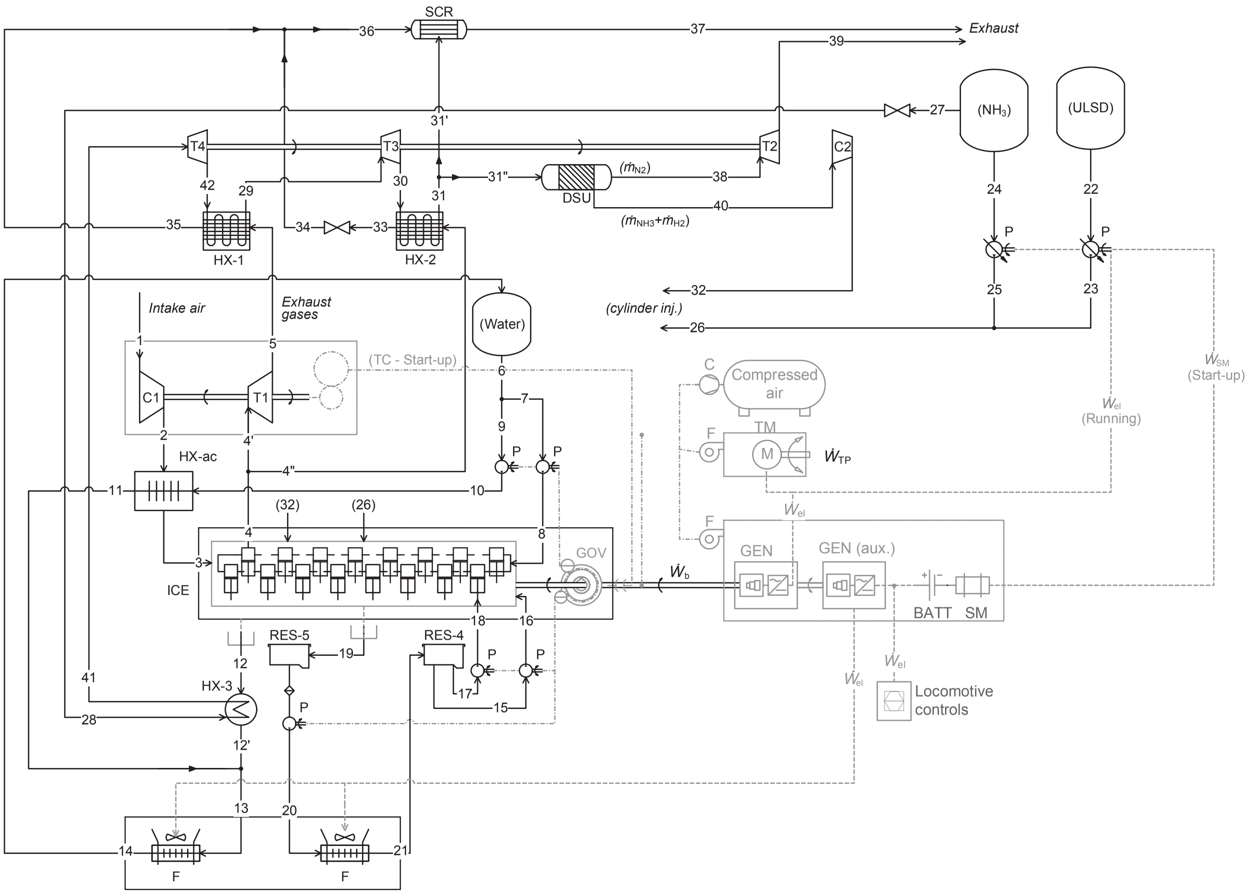


Fig. 6.11 Integrated engine cooling

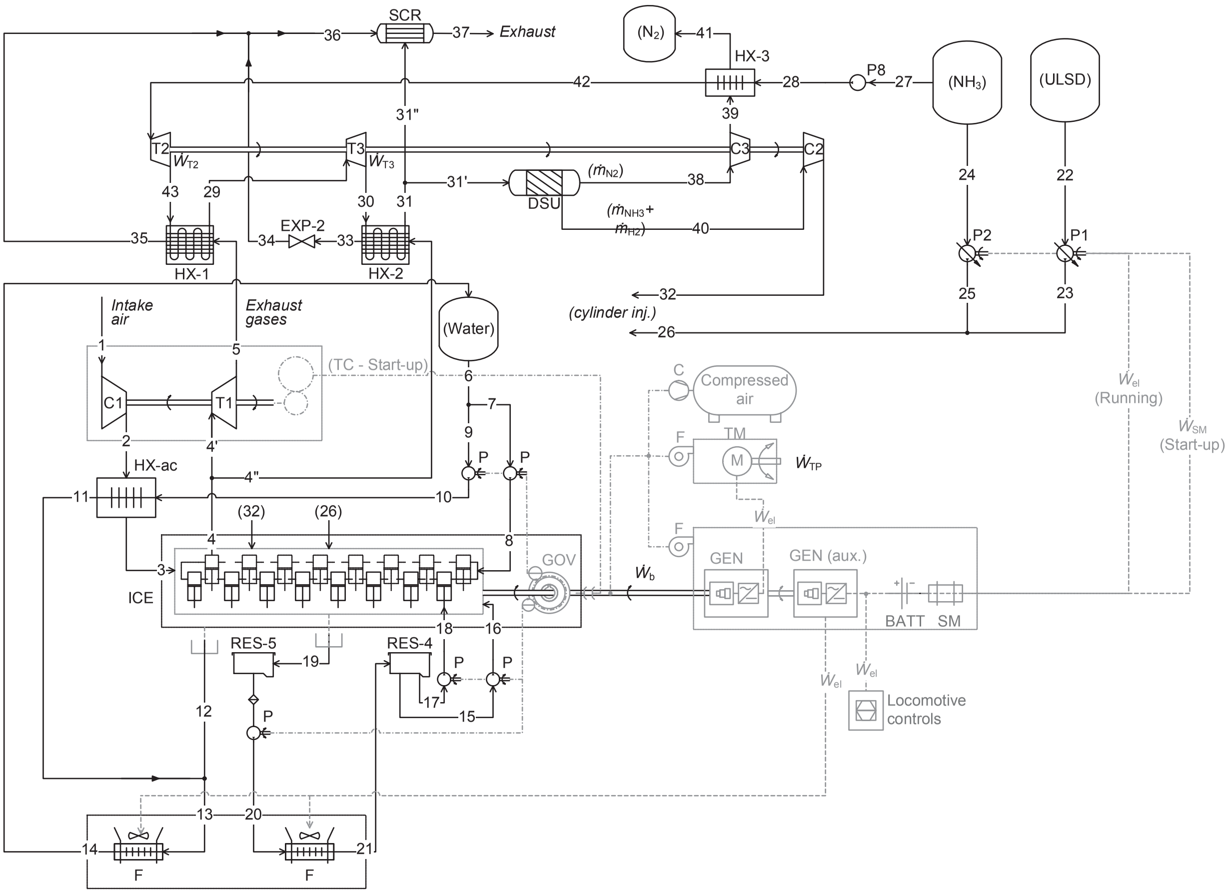


Fig. 6.12 Integrated compressed nitrogen gas storage

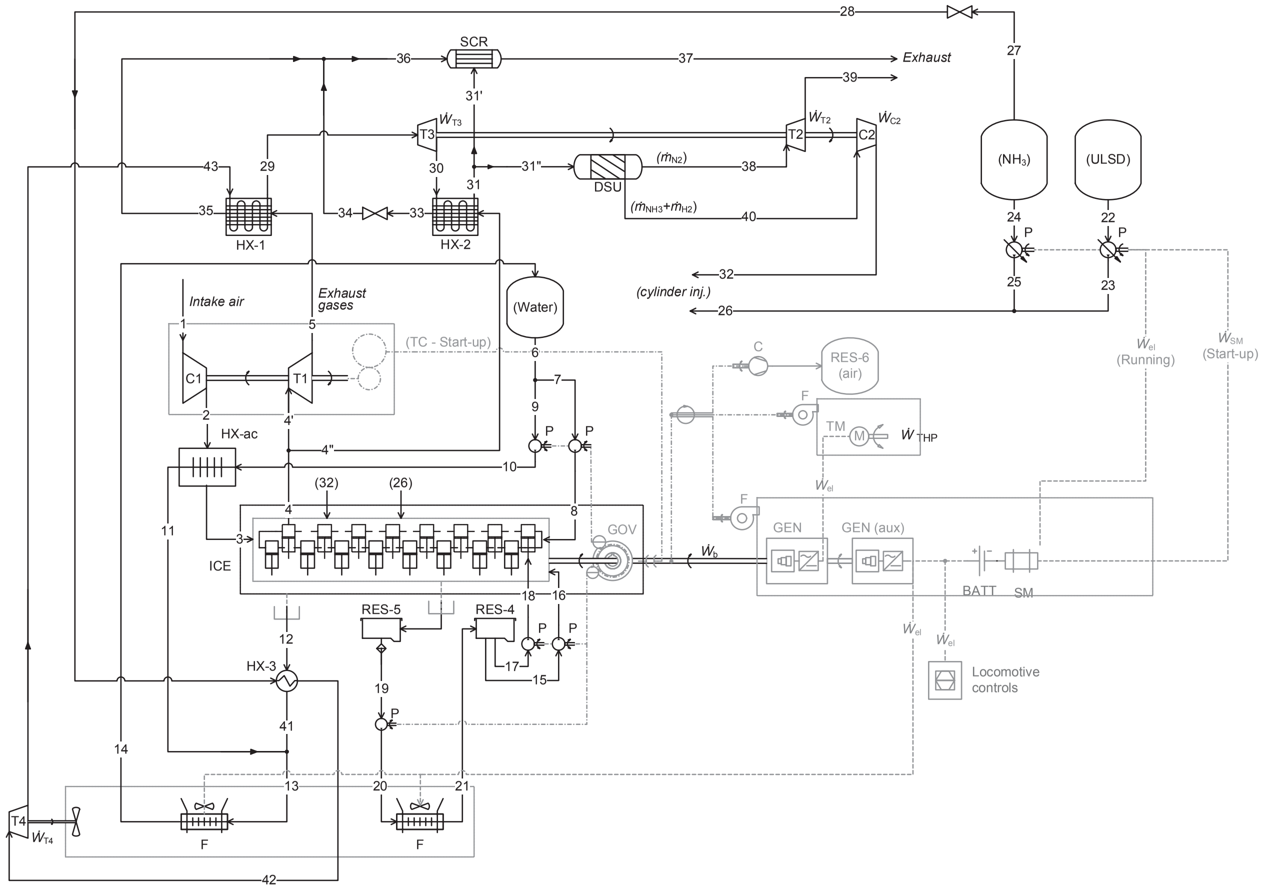


Fig. 6.13 Indirect engine cooling

supply streams. N_2 gas is expanded in T2. NH_3–H_2 stream is compressed in C2 to be injected into the ICE with ULSD.

6.11 System 9: Integrated Ammonia-Based Cab Cooling System

The configuration shown in Fig. 6.14 includes the additional ammonia process of cab cooling. Ammonia is throttled to an intermediate pressure level, with a low temperature useful for cooling. The cold stream of ammonia is circulated through a chiller (CH), assumed to be filled with water. Chilled water is circulated in an air-cooling heat exchanger (HX-4), which allows the cooling to be on demand for the operator and can be controlled by a fan. The cool stream of ammonia leaves the chiller tank, and is used to provide cooling for the engine jacket water in HX-3. The warm ammonia is then superheated in HX-1 and expanded in T3 before being re-superheated (HX-2) and decomposed in the DSU. As in the previous system, a portion of the ammonia stream is diverted to the SCR to reduce engine NO_x. The gas mixture leaving the DSU is not separated, and instead it is compressed (C2) and sent as a mixture with ULSD for combustion in the ICE. The cooling system is assumed to have an overall COP of 2.0, which is the same assumption as other engine cooling processes for the locomotive. The temperature of the cold stream is kept above 0 °C, to ensure that there is no ice formation in the water. Alternatively, the tank could hold brine or other mixtures, which have lower freezing points to improve the cooling performance.

6.12 System 10: Heat Recovery NH_3–Rankine Cycle

In the configuration shown in Fig. 6.15, a heat engine operating as a Rankine cycle is integrated with the system, the NH_3 fuel stream used as the working fluid cycle. The liquid NH_3 stream is pumped to the exhaust heat recovery exchanger HX-4, which serves as the boiler component for the NH_3–Rankine cycle (NH_3–RC) heat engine. Vapor produced in the heat recovery process (either saturated vapor or superheated) is expanded in turbine T5 to produce shaft work and is then condensed in HX-5 by transferring heat to the secondary NH_3 stream. The condensed NH_3 is then mixed with the ULSD stream and is fed into the ICE for combustion.

The secondary NH_3 stream is drawn from the tank and throttled to a lower pressure liquid–vapor mixture. The stream recovers heat in HX-5, and the vapor is expanded in T4 to produce work. The intermediate pressure NH_3 is reheated in HX-1 and then expanded to a lower pressure level in T3. The stream is reheated in HX-2, and the required supply rate of NH_3 sent through the SCR for NO_x reduction. Following the decomposition process, N_2 gases are fed through the final expansion pro-

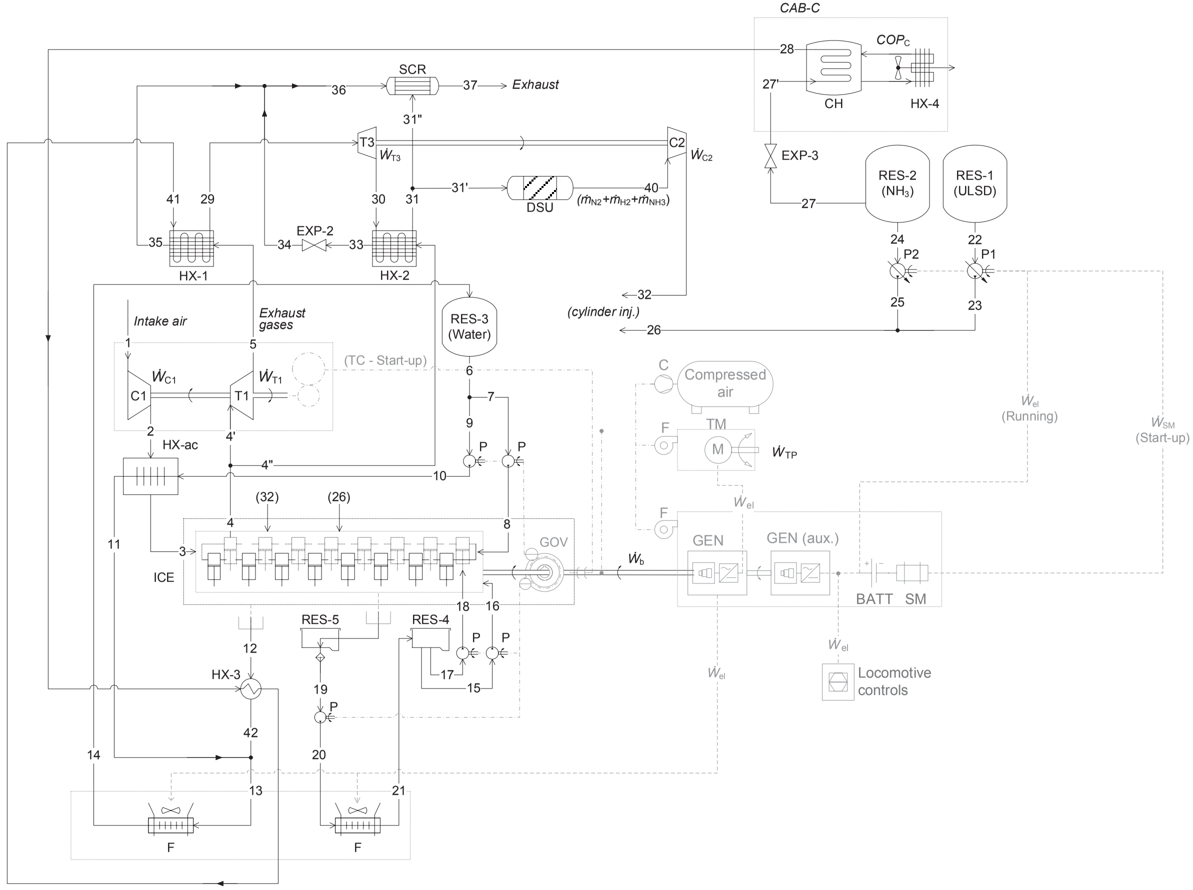


Fig. 6.14 Integrated ammonia-based cab cooling system

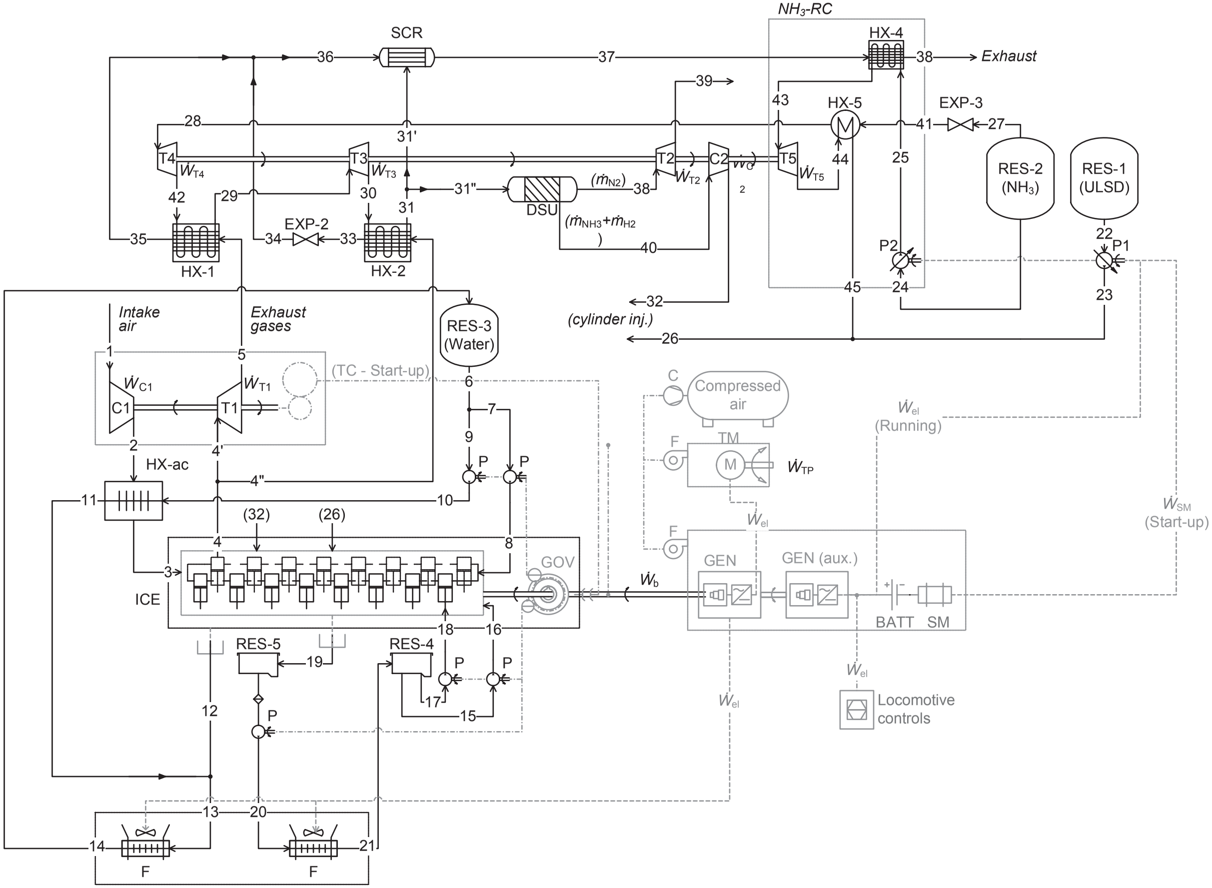


Fig. 6.15 Heat recovery NH_3–rankine cycle

cess in T2, and the H_2 stream is compressed to be injected into the ICE with ULSD. The remaining NH_3 gas is cooled and pumped back to the storage tank.

6.13 Closing Remarks

Integrated systems utilizing ammonia in various fueling, heat recovery, and cooling subsystem applications are discussed in this chapter. The systems take into consideration green engineering design principles: reducing nonrenewable (i.e., fossil fuel) inputs by supplying ammonia fuel, reducing system losses in the form of heat to more effectively utilize the fuel energy supplied to the prime mover engine, and addressing opportunities for energy recovery with additional power generation where possible by taking advantage of the thermophysical properties of ammonia to generate power with low-temperature heat sources.

By integrating ammonia throughout the locomotive prime mover systems, we can take advantage of its applicability as a combustion fuel, heat transfer fluid/engine coolant, and working fluid in cooling processes. Furthermore, it is possible to significantly reduce the diesel fuel requirement, energy demand to power and carry large cooling fans and heat exchangers by reducing the required sizing, reduce the heat losses, and reduce the environmental impact of diesel fuel combustion.

Chapter 7
Locomotive Systems Analyses and Assessment

7.1 Introduction

Transportation—as any other human activity—is bounded to physical laws which manifest in the surroundings environment. The speed of a vehicle is limited to certain value depending on the medium through which it travels, friction effects, materials used in vehicle construction, type of engine, and fuels. The transportation sector with its roads, routes, railways, and vehicles reshapes continuously as driven by the actual needs of societies and as bounded by the current knowledge and the laws of thermodynamics.

It is of major importance to develop tools for analysis and assessment of the transportation sector and its components. Thermodynamic analysis must stand at the base of any assessment activity due to its systemic approach. Very common is the thermodynamic analysis and assessment through energy method. Energy is conserved, and due to this fact, it can be inventoried. Figures of merit such as efficiency, fuel optimization factor, and specific fuel consumption can be assigned to any type of vehicle or transportation system. These figures of merit may allow for a comparative assessment of transportation systems.

However, a more objective assessment is obtained when the systems' irreversibilities are accounted for. Other feature aspects must be also included in the analyses so that the systems can be assessed based on environmental and economic criteria besides efficiencies. In this chapter, we aim to provide a right-to-the-point-type approach to introduce thermodynamic aspects of cycles and locomotive systems under the first law of thermodynamics (FLT) and second law of thermodynamics (SLT) to write the main balance equations for mass, energy, entropy, and exergy and define two key efficiencies as energy and exergy efficiencies for performance assessment and evaluation. These are specifically driven for the locomotive systems' design, analysis, and assessment and become the base for the case studies of the present developed systems which are presented in Chap. 8

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DOI 10.1007/978-3-319-21726-0_7

7.2 Thermodynamic Aspects

The concept of system is critical in thermodynamics and necessary for thermodynamic design, analysis, and assessment. A thermodynamic system represents a fictive delimitation of a region of space subjected to the analysis. When a system is defined, its surrounding is automatically described. A thermodynamic system can interact with its surrounding through mass transfer, work transfer, or heat transfer. Work transfer represents a perfectly organized energy transfer. On the contrary, heat carries chaos and therefore transfers entropy besides energy. The internal energy of a system represents a state function defined as a potential to do work. The total energy within a system is a sum of multiple energy forms that may be accumulated within the system's boundary, including the internal energy. In system analysis, writing balance equations correctly is the most critical step and should be written accordingly after defining the system boundary to identify all inputs and outputs. One should then write mass balance equation (MBE), energy balance equation (EBE), entropy balance equation (EnBE), and exergy balance equation (ExBE), respectively.

Based on the concepts of heat, work, and energy, the FLT can be formulated. This law states that energy is conserved, or as paraphrased "you can't get something from nothing." As shown in Fig. 7.1, the FLT can be expressed in a compact form as an EBE. As seen, the EBE can be expressed as simply as $E_{\mathrm{in}} = \Delta E_{\mathrm{sys}} + E_{\mathrm{out}}$.

Furthermore, the EBE can be expressed for an open system in rate form as follows:

$$\sum_{\mathrm{in}} \dot{m}h + \sum_{\mathrm{in}} \dot{Q} + \sum_{\mathrm{in}} \dot{W} = \frac{\mathrm{d}E_{\mathrm{sys}}}{\mathrm{d}t} + \sum_{\mathrm{out}} \dot{m}h + \sum_{\mathrm{out}} \dot{Q} + \sum_{\mathrm{out}} \dot{W}. \tag{7.1}$$

Regarding the *SLT,* this provides a mean to predict the direction of any process in time, to establish conditions of equilibrium, to determine the maximum attainable performance of machines and processes, to assess quantitatively the irrevers-

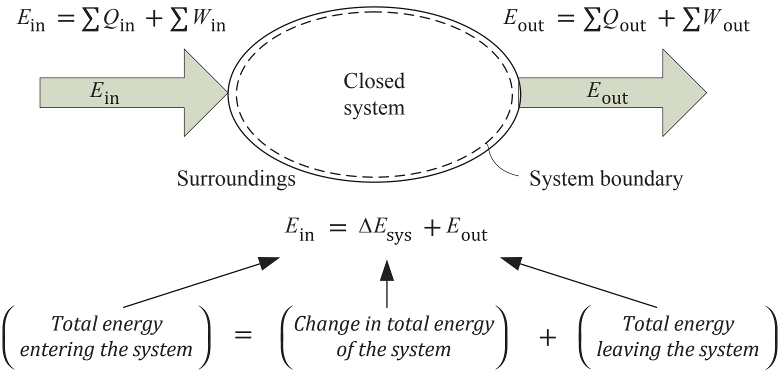

Fig. 7.1 Illustrating the energy balance equation for a closed system

ibilities, and to determine their magnitude for the purpose of identifying ways of improvement of processes. The SLT is related to the concepts of reversibility and irreversibility. One says that a thermodynamic process is reversible if during a transformation both the thermodynamic system and its surroundings can be returned to their initial states. Reversible processes are of three kinds and are as follows:

- *Externally reversible*—with no associated irreversibilities outside the system boundary.
- *Internally reversible*—with no irreversibilities within the boundary of the system during the process.
- *Totally reversible*—with no irreversibilities within the system and surroundings.

The SLT is a useful tool in predicting the limits of a system to produce work while generating irreversibilities to various imperfections of energy conversion or transport processes. The most fundamental device with cyclical operation in thermodynamics is heat engine; other important device is heat pump.

These devices operate between a heat source and a heat sink. A heat sink represents a thermal reservoir capable of absorbing heat from other systems. A heat source represents a thermal reservoir capable of providing thermal energy to other systems. A heat engine operates cyclically by transferring heat from a heat source to a heat sink. While receiving more heat from the source (Q_H) and rejecting less to the sink (Q_C), a heat engine can generate work (W). As stated by the FLT, energy is conserved; thus, $Q_H = Q_C + W$.

A typical "black box" representation of a heat engine is shown in Fig. 7.2a. According to the SLT, the work generated must be strictly lesser than the heat input, $W < Q_H$. The thermal efficiency of a heat engine—also known as energy efficiency—is defined as the net work generated by the total heat input. Using notations from Fig. 7.2a, energy efficiency of a heat engine is expressed (by definition) with

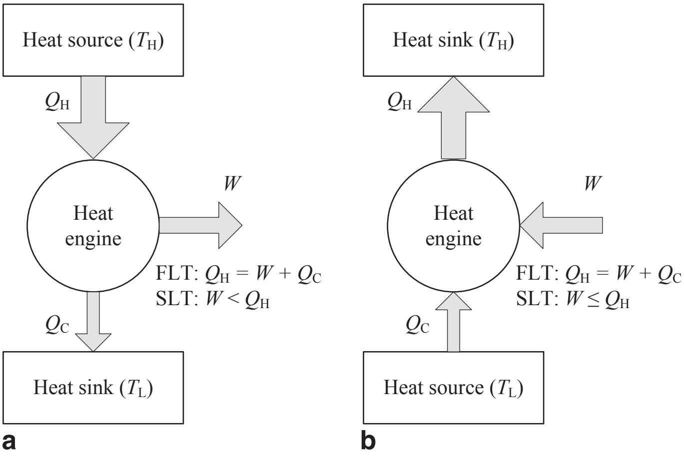

Fig. 7.2 Conceptual representation of a heat engine (**a**) and heat pump (**b**)

$$\eta = \frac{W}{Q_{\mathrm{H}}} = 1 - \frac{Q_{\mathrm{C}}}{Q_{\mathrm{H}}} \tag{7.2}$$

If a thermodynamic cycle operates as refrigerator or heat pump, then its performance can be assessed by the *coefficient of performance (COP)* defined as useful heat generated per work consumed. As observed in Fig. 1.11b, EBE for a heat pump is written as $Q_{\mathrm{C}} + W = Q_{\mathrm{H}}$; according to SLT, $Q_{\mathrm{H}} \geq W$ (this means that work can be integrally converted to heat). Based on its definition, the COP is written as

$$\mathrm{COP} = \frac{Q_{\mathrm{H}}}{W} = \frac{Q_{\mathrm{H}}}{Q_{\mathrm{C}} + W} \tag{7.3}$$

The Carnot cycle is a fundamental model in thermodynamics representing a heat engine (or heat pump) that operates between a heat source and a heat sink, both of them being at constant temperature. This cycle is a conceptual (theoretical) cycle and was proposed by Sadi Carnot in 1824. The cycle comprises fully reversible processes, namely two adiabatic and two isothermal processes. The efficiency of Carnot cycle is independent of working fluid which performs cyclically the processes. The energy efficiency of a reversible Carnot heat engine is defined as:

$$\eta = 1 - \frac{T_{\mathrm{L}}}{T_{\mathrm{H}}} \tag{7.4}$$

and the COP of the reversible Carnot heat pump becomes

$$\mathrm{COP} = \frac{T_{\mathrm{H}}}{\left(T_{\mathrm{H}} - T_{\mathrm{L}}\right)} \tag{7.5}$$

and the COP of the reversible Carnot refrigerator becomes

$$\mathrm{COP} = \frac{T_{\mathrm{L}}}{\left(T_{\mathrm{H}} - T_{\mathrm{L}}\right)} \tag{7.6}$$

using the temperature scale as $(Q_{\mathrm{H}}/Q_{\mathrm{L}})_{\mathrm{rev}} = (T_{\mathrm{H}}/T_{\mathrm{L}})$.

In summary, the above given Carnot efficiency and Carnot COPs are useful criteria to assess practical heat engines, refrigerators, heat pumps, or other energy conversion systems with respect to the idealized case of reversible devices. Accordingly, energy efficiency *(η)* and COP of a reversible thermodynamic cycle are highest possible and any actual (irreversible) cycle has smaller efficiency ($\eta_{\mathrm{rev}} > \eta_{\mathrm{irrev}}$) and ($\mathrm{COP}_{\mathrm{rev}} > \mathrm{COP}_{\mathrm{irrev}}$).

Exergy represents the maximum work which can be produced by a thermodynamic system when it comes in equilibrium with its surroundings environment. This statement assumes that at an initial state, there is a thermodynamic system which is not in equilibrium with the environment. In addition, it is assumed that—at least potentially—mechanisms of energy (and mass) transfer between the system and the environment must exist—such that eventually such equilibrium condition will occur in the system.

The system must at least exchange work with the environment. Another remark is that exergy definition assumes the existence of a reference environment. The system under the analysis will interact only with that environment. Exergy analysis is a method appertaining to engineering thermodynamics and can be used to determine the alleviation of man-made and natural systems from the ideal case. Here, by ideal system one understands a reversible system.

Exergy cannot be conserved. Any real process destroys exergy as it generates entropy. Exergy is destroyed and entropy is generated due to irreversibilities. The exergy of a closed (non-flow) thermodynamic system comprises four terms, namely physical (or thermomechanical), chemical, kinetic, and potential. In brief, the total exergy of a non-flow system is written as:

$$Ex_{\mathrm{nf}} = Ex_{\mathrm{ph}} + Ex_{\mathrm{ch}} + Ex_{\mathrm{ke}} + Ex_{\mathrm{pe}} \tag{7.7}$$

The exergy of a flowing stream of matter Ex_{f} represents the sum of the non-flow exergy and the exergy associated with the flow work of the stream $(P - P_0)V$; therefore,

$$Ex_{\mathrm{f}} = Ex_{\mathrm{nf}} + (P - P_0)V \tag{7.8}$$

The physical exergy for a non-flow system is defined by

$$Ex_{\mathrm{ph}} = (U - U_0) + P_0(V - V_0) - T_0(S - S_0) \tag{7.9}$$

where U is internal energy, V is volume, S is entropy of closed system which is in nonequilibrium with the environment, T_0 is the reference temperature of the surroundings environment, and index 0 refers to the values of the parameters when the system is in thermomechanical equilibrium with the environment.

If a substance is not present in the atmosphere then the reference for zero chemical exergy is the most stable state of that substance in seawater. There are developed tables of chemical exergy of elements in past literature data. Standard chemical exergy of elements is useful for the calculation of chemical exergy of chemical compounds provided that their Gibbs energy of formation is known.

Moreover, if system compounds have other concentration or other phase as that corresponding to the environment, then various processes such as dilution or concentration may occur until there is no difference in concentration between system components and the environment.

The chemical exergy depends on the difference between chemical potential of system components $\left(\sum n_{\mathrm{i}} \mu_{\mathrm{i}}^{0}\right)$ being in thermomechanical equilibrium but not in chemical equilibrium with it (μ_{i}^{0}), and the chemical potential of system components (μ_i^{00}) when they are brought in chemical equilibrium with the environment $\left(\sum n_i \mu_i^{00}\right)$. Therefore, the chemical exergy of the system is defined as

$$Ex_{ch} = \sum n_i \left(\mu_i^0 - \mu_i^{00}\right) \tag{7.10}$$

It is important to analyze the chemical exergy due to concentration difference between the system and the surroundings environment. Let us assume the thermodynamic system at state 1 in nonequilibrium with the environment. If mass transfer is permitted with the environment, a dilution process occurs until the moment when the system components are fully diluted and there is no concentration gradient; this state is denoted as 2. The maximum work extractable from process 1 to 2 represents the exergy due to concentration difference and is given by

$$\begin{aligned} \Delta\, Ex_{conc}^{ch} &= Ex_1 - Ex_2 \\ &= \left(U_1 - U_2\right) + \left(P_1V_1 - P_2V_2\right) - T_0\left(S_1 - S_2\right) \\ &= T_0(S_2 - S_1) \end{aligned} \tag{7.11}$$

Here, one accounts that the process of diffusion is isothermal and one assumes that the gases involved are ideal gas $U_2 = U_1$ and $P_2V_2 = P_1V_1$. Furthermore, according to the FLT, $T\ \mathrm{d}S = \mathrm{d}U + P\ \mathrm{d}V$; therefore, for an isothermal process of ideal gas for which $\mathrm{d}U = 0$ and $\mathrm{d}(P\,V) = 0$, one has $T\ \mathrm{d}S = \mathrm{d}(P\ V) - v\ \mathrm{d}P$ or $T\mathrm{d}S = -v\mathrm{d}P$. Consequently, the chemical exergy due to difference in concentration of the gas component i having molar fraction y_i is given as follows:

$$Ex_{conc,i}^{ch} = -RT_0 \ln\left(y_i\right) \tag{7.12}$$

The notion of *Gibbs free energy* is introduced as a *state function* defined by $g = h - Ts$; this function can be used to determine the maximum work related to chemical processes. In order to determine the chemical exergy of a compound, it is required to know its standard Gibbs free energy of formation, $\Delta^f g^0$. Then, using $\Delta^f g^0$ and the standard exergy of the elements, the following formula must be used to determine the chemical exergy of the compound:

$$ex^{ch} = \Delta^f g^0 + \sum_{element} \left(\nu\ ex^{ch}\right)_{element} \tag{7.13}$$

where v is the stoichiometric factor representing the number of moles of element per one mole of chemical compound.

An example of chemical exergy calculation is given here for methane. The formation reaction of methane is $C + 2H_2 \rightarrow CH_4$, while the standard formation Gibbs energy is $\Delta^f g^0 = -50.53$ kJ/mol. The standard chemical exergy of hydrogen is 236.12 kJ/mol, while that of carbon (graphite) is 410.27 kJ/mol. Therefore, the chemical exergy of methane is computed as follows: $ex_{CH4}^{ch} = -50.53 + 410.27 + 2 \times 236.12 = 832\ \mathrm{kJ/mol}$.

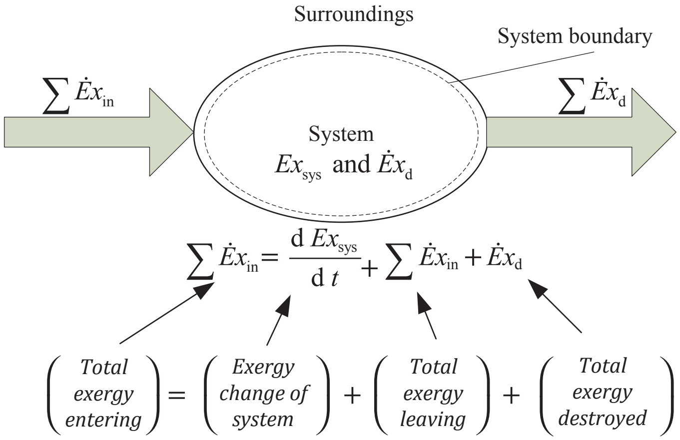

Fig. 7.3 Explanatory sketch for the exergy balance equation

The ExBE introduces the term *exergy destroyed* which represents the maximum work potential that cannot be recovered for useful purpose due to irreversibilities.

For a reversible system, there is no exergy destruction since all work generated by the system can be made useful. The exergy destruction and entropy generation are related by the expression $Ex_{\text{d}} = T_0\ \Delta\, S_{\text{gen}}$, where T_0 is the reference temperature. If $Ex_{\text{d}} > 0$, then the process is irreversible; if $Ex_{\text{d}} = 0$, then the process is reversible; and if $Ex_{\text{d}} < 0$, the process is impossible.

The total exergy entering a thermodynamic system must be balanced by the total exergy leaving the system plus the change of exergy content of the system plus the exergy destruction. Figure 7.3 shows an explanatory sketch for the ExBE.

Exergy can be transferred to or from a system by three means: work, heat, and mass. Therefore, the ExBE can be expressed generally in rate form as follows:

$$\begin{aligned}\text{ExBE}: &\sum_{\text{in}} \left[\dot{W} + \dot{m}\varphi + \left(1 - \frac{T_0}{T}\right)\dot{Q}\right] \\ &= \frac{\mathrm{d}Ex_{\text{sys}}}{\mathrm{d}t} + \sum_{\text{out}} \left[\dot{W} + \dot{m}\varphi + \left(1 - \frac{T_0}{T}\right)\dot{Q}\right] - P_0 \frac{\mathrm{d}V_{\text{CV}}}{\mathrm{d}t} + \dot{E}x_{\text{d}}\end{aligned} \tag{7.14}$$

where the *total specific exergy* is $\varphi = (h - h_0) + T_0(s - s_0) + \frac{1}{2}v^2 + g(z - z_0) + ex^{\text{ch}}$.

Exergy transfer between the system and surrounding can be done by work transfer, mass transfer, and heat transfer. The exergy due to work transfer (Ex^{W}) is, by definition, equal to the work: $Ex^{\text{W}} = W$. However, if the system impinges against a moving boundary, then the exergy must be diminished accordingly; thus, $Ex^{\text{W}} = W - P_0(V - V_0)$. The exergy associated with mass transfer (Ex^{m}) is $Ex^{\text{m}} = m\ \varphi$. The exergy due to heat transfer can be expressed based on Carnot factor according to the following equation:

$$Ex^{\mathrm{Q}} = \int\limits_{\substack{system\\boundary}} \left(1 - \frac{T_0}{T}\right) \mathrm{d}Q \tag{7.15}$$

The term efficiency originates mainly from thermodynamics when the attempt of assessing the heat conversion into work leads to its initial formulation as the "work generated per total heat energy input." However, efficiency as assessment criterion can be applied widely for any system and process. A general efficiency expression of a system—as a measure of its performance and effectiveness—is represented by the ratio of useful output per required input. Here, it is recognized as an efficiency criterion based on FLT, also called *energy efficiency*. If the system is an energy system, then its input and output must be forms of energy. Therefore, for an energy system, the energy efficiency is written as

$$\eta = \frac{\dot{E}_{\mathrm{deliv}}}{\dot{E}_{\mathrm{cons}}} = 1 - \frac{\dot{E}_{\mathrm{loss}}}{\dot{E}_{\mathrm{cons}}}. \tag{7.16}$$

Any source of energy stream is characterized by an associated exergy. By analogy with energy efficiency, the exergy efficiency is defined as the ratio between exergy associated with the useful output and the exergy associated with the consumed input, namely:

$$\psi = \frac{\dot{E}x_{\mathrm{deliv}}}{\dot{E}x_{\mathrm{cons}}} = 1 - \frac{\dot{E}x_{\mathrm{d}}}{\dot{E}x_{\mathrm{cons}}}. \tag{7.17}$$

7.3 Thermodynamic Power Cycles

Power cycles are loop processes which, within a fluid, follow certain transportations as repeated in a cycle, with power generation being the net effect. The power cycles can be categorized as vapor and gas power cycles. In gas power cycles, the working fluid does not experience any liquid–vapor transformation process (boiling, condensation) like in vapor power cycles. Rather, the working fluid in gas power cycles remains in a gaseous state of aggregation during all cycle's processes. There are three types of totally reversible power cycles, these being Carnot, Stirling, and Ericsson. There are three main types of internally reversible power cycles, namely Otto, Diesel, and Brayton. The vapor power cycles are also known as Rankine cycles and can operate with various fluids including steam, organic fluids, and inorganic fluids such as carbon dioxide.

The very condition for a cycle to be totally reversible is that its heat addition and rejection processes should be isothermal. If the heat addition and rejection processes are not isothermal, then the cycle must be externally irreversible because a finite temperature difference must occur between a thermal reservoir at fixed temperature and the working fluid. Carnot, Stirling, and Ericsson cycles include two isothermal heat addition processes. The other two processes (from a total of four) are adiabatic for Carnot cycle, isochoric for Stirling cycle, and isobaric for Ericsson cycle. The efficiency of any totally reversible heat engine (e.g., Carnot, Stirling, and Ericsson) connected to a heat source of temperature T_H and to a heat sink of temperature T_L is given by the Carnot factor.

The fundamental thermodynamic cycles that are internally reversible are Brayton, Otto, and Diesel. All these cycles are a good choice for internal combustion engines (ICEs) and thus for engine-driven power generators. Brayton cycle has been extensively analyzed in previous two sections. This cycle is better suited for large-scale power generation in combined cycle power plants. Here the Otto, Diesel, and the so-called dual cycles are analyzed in detail. These cycles are the most common for engine-driven generators which consist of an internal combustion engine installed on the same chassis with an electrical generator and a power regulation block. Applications of engine-driven power generators can be both stationary and portable (mobile).

7.3.1 Otto Cycle

The Otto cycle is the ideal cycle for spark ignition engines. This cycle has been established in 1870s after the successful demonstration of the four-stroke spark ignition engine by Nikolaus Otto. The cycle and the processes are presented in Fig. 7.4

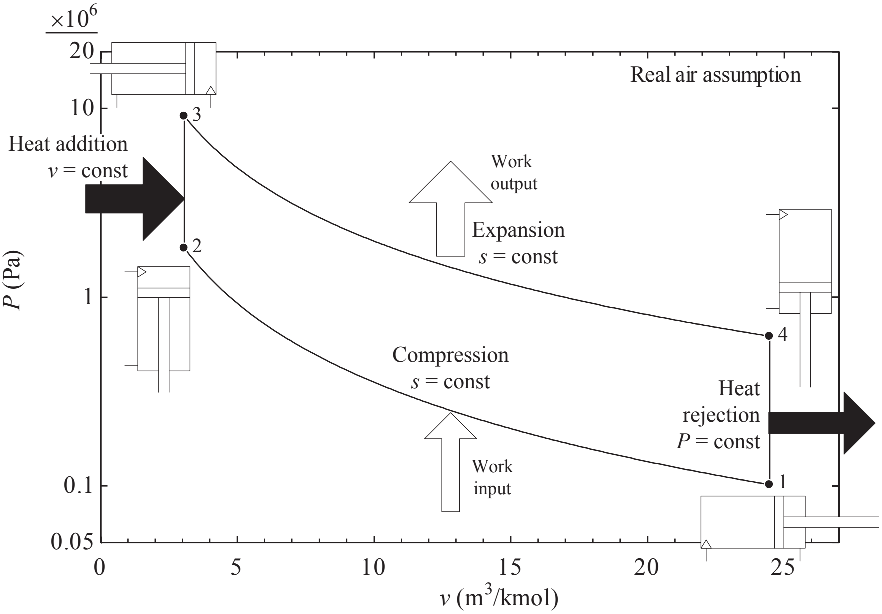

Fig. 7.4 Ideal Otto cycle under real air assumption for $r_v = 8, r = 90$

where the piston–cylinder operation and the $P-v$ diagram are illustrated. The cycle consists of two isentropic and two isochoric processes of a gas. The numerical example taken in the diagram is for a volume ratio $r_{\mathrm{v}} = v_1 / v_2 = 8$ and a pressure ratio $r = P_3 / P_1 = 90$. As it will be shown subsequently, for these conditions, the energy efficiency with real air as working fluid is 47.3 %, while the exergy efficiency is 51.9 % and Carnot factor is 0.911.

In thermodynamic state 1, there is a gas enclosed in a cylinder in thermal equilibrium with the low-temperature reservoir at $T_1 = T_0$. The processes are given as follows:

- Isentropic compression, process 1–2: The piston is moved leftward and compresses the gas while at the same time, the cycle receives work from the outside. The process is isentropic and adiabatic.
- Isochoric heat addition, process 2–3: The piston remains in fixed position while heat is added to the working fluid. In internal combustion engine, this heat is due to a combustion process (with spark ignition). The temperature and pressure of the gas increase considerably during the isochoric heat addition process.
- Isentropic expansion, process 3–4: The piston moves down (see the figure) and produces a motor strokes that generates usable work. The expansion continues until the volume reaches the maximum stroke when $v_4 = v_1$.
- Isochoric heat removal, process 4–1: The piston remains in fixed position while heat is removed from the gas by placing the gas in thermal contact with the heat sink. In practical applications with internal combustion engine, during process 4–1 the heat is removed by expelling out the gas to the atmosphere while allowing fresh air in.

The Otto cycle is externally irreversible because its heat addition and removal processes are not isothermal. Therefore, the efficiency of this cycle is lower than that given by the Carnot factor. Under the standard air assumption, an analytical expression for the cycle efficiency can be derived. During the isochoric processes, there is no work exchange with the surroundings. Therefore, the isentrope equations $T_2 = r_{\mathrm{v}}^{\gamma-1} T_1$ and $T_3 = r_{\mathrm{v}}^{\gamma-1} T_4$ require that the efficiency of the internally reversible Otto cycle is

$$\eta = 1 - \frac{Q_{\mathrm{out}}}{Q_{\mathrm{in}}} = 1 - \frac{T_4 - T_1}{T_3 - T_2} = 1 - r_{\mathrm{v}}^{1-\gamma}. \tag{7.18}$$

The exergy efficiency of the cycle results from an exergy balance in which it is assumed that the sink temperature is the same as the reference temperature T_0. The following equation for the exergy efficiency results:

$$\psi = \frac{\dot{W}_{\mathrm{net}}}{Ex_{\mathrm{in}}} = \frac{\dot{W}_{\mathrm{net}}}{\dot{Q}_{\mathrm{n}} \left(1 - \frac{T_0}{T_{\mathrm{so}}}\right)} = \frac{\eta}{1 - \frac{T_0}{T_{\mathrm{so}}}}. \tag{7.19}$$

7.3.2 Diesel Cycle

Diesel cycle is used in many application of industrial-scale power generation where large engine generator groups can be installed. The engines which are based on Diesel cycle are denoted as compression ignition ICEs. This thermodynamic cycle and the compression ignition engine were proposed in Germany by Rudolf Diesel around 1895. In this type of engine, the ignition of the combustion process is obtained by compressing the air up to a temperature superior to the autoignition of the fuel. The moment air reaches sufficiently high temperature, pressurized liquid fuel is injected into the cylinder and the ignition process occurs instantly. An ideal Diesel cycle is shown in Fig. 7.5.

Because air temperature must be sufficiently high (over 800 K), the volume ratio (also called compression ratio) for Diesel cycle must be in the typical range of $r_v = 12$ to 24. Since no spark is given to initiate combustion process in compression ignition engine, the duration of the combustion is relatively slow. Consequently, the pressure can be kept almost steady provided that the injection occurs at top dead center (TDC—the upmost position of the piston). Since the volume increases during the combustion, the temperature of the gases will follow this increase. Figure 5.45 presents an ideal Diesel cycle. It comprises the following processes:

- Isentropic compression, process 1–2: The gas entrapped in the cylinder is compressed adiabatically by moving the piston leftward. Work consumption is required.

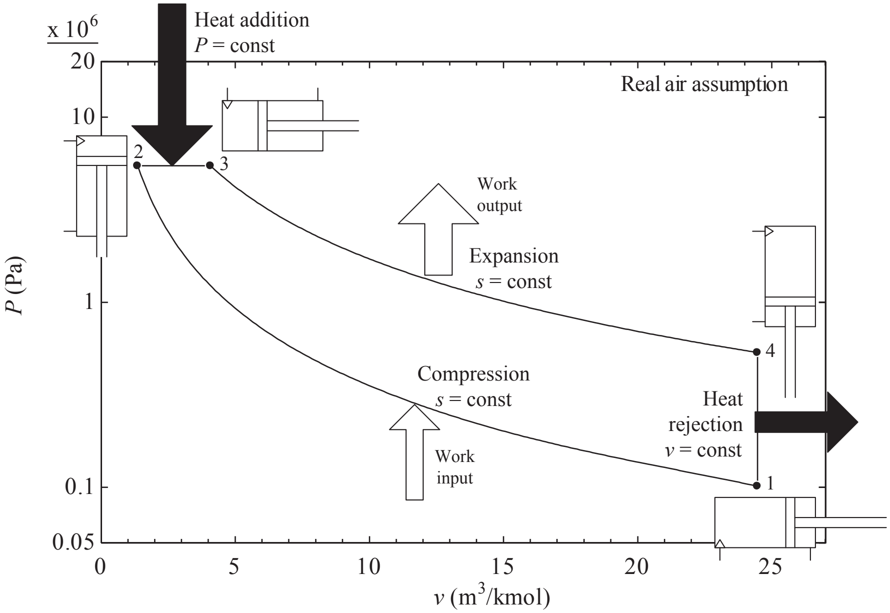

Fig. 7.5 Ideal Diesel cycle under real air assumption for $r_v = 18, r_c = 3$

- Isobaric heat addition, process 2–3: During the heat addition process, the pressure is maintained constant by increasing the cylinder volume. The temperature of the gas increases due to the heat addition process.
- Isentropic expansion, process 3–4: This is the motor stroke when the piston produces useful work. The expansion stroke stops when $v_4 = v_1$.
- Isochoric heat removal, process 4–1: Heat is rejected while the cylinder volume remains constant. This process is similar to that described for Otto cycle above.

It is easy to demonstrate that the efficiency of air-standard Diesel cycle is given by the following equation:

$$\eta = 1 - \frac{1}{\gamma r^{\gamma-1}} \frac{r_c^{\gamma} - 1}{r_c - 1} \tag{7.20}$$

7.3.3 Dual Cycle

The ideal dual cycle, shown qualitatively in Fig. 7.6, consists of four major processes: isentropic compression (1–2), heat addition (2–4A), isentropic expansion (4–5), and constant volume heat rejection (5–1). Heat addition occurs in two stages: constant volume (2–3A) and constant pressure (3A–4A). Figure 7.6a represents the cycle in the *P–V* diagram, whereas the *T–s* diagram is shown in Fig. 7.6b. As it results from these figures, the dual cycle fits in between the Diesel and Otto cycles. The peculiarity of the dual cycle is that its heat addition process is in part at constant volume (such as in Otto) and in part at constant pressure (such as in Diesel).

As a consequence, the upper pressure and temperature within the ideal dual cycle are higher than for Diesel and lower than for Otto, provided that all cycles operate between the same cylinder volume limits (i.e., the same compression ratio *r*), as shown in Fig. 7.6.

The cycle model is based on the known engine geometry and operating characteristics such as compression ratio *(r)*, cylinder volumes *(V_i)*, rated traction power,

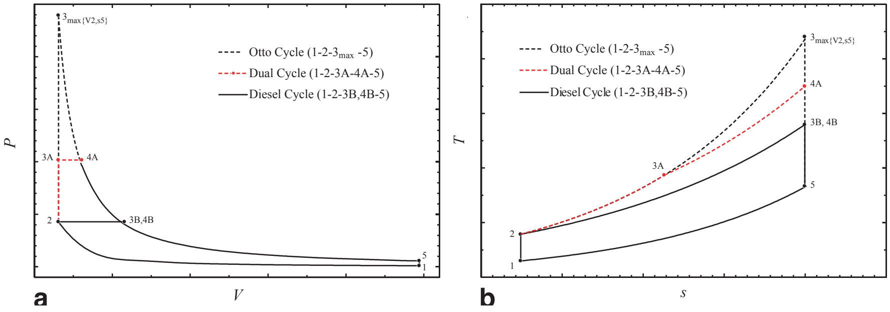

Fig. 7.6 Air-standard qualitative *P–V* (**a**), and *T–s* (**b**) diagrams of the dual cycle

Table 7.1 Dual cycle modeling equations (γ = constant)

State points	Process	Equations
1–2	Isentropic compression	$P_2 = P_1 r^{\gamma}$ $T_2 = T_1 r^{(\gamma-1)}$
2–4	Heat addition at constant volume and constant pressure	$\dot{Q}_{2-3} = \dot{m}_{\text{exh}} C_{\text{v}}(T_3 - T_2)$ (constant volume process, $V_2 = V_3$) $\dot{Q}_{3-4} = \dot{m}_{\text{exh}} C_{\text{p}}(T_4 - T_3)$ (constant pressure process, $P_3 = P_4$) $\dot{Q}_{\text{in}} = \dot{Q}_{2-3} + \dot{Q}_{3-4}$
4–5	Isentropic expansion	$P_5 = P_4 r^{-\gamma}$ $T_5 = T_4 r^{-(\gamma-1)}$
5–1	Heat rejection at constant volume	$\dot{Q}_{5-1} = \dot{m}_{\text{exh}} C_{\text{v}}(T_5 - T_1)$

and maximum cylinder pressure ($P_{\text{max}} = P_3$). The equations describing the cycle processes are outlined in Table 7.1. The model involves the assumption that the specific heat ratio γ is constant. In general, for dual cycle modeling, the specific heat ratio of combustible gases is taken as $\gamma = 1.35$. As seen in the table, the equations for pressure and temperature change along an isentropic process and are used to model the compression and expansion. For heat rejection, the specific heat at constant volume is involved in the EBE. For the heat addition process, both specific heats—at constant pressure and at constant volume—are required for the modeling.

7.3.4 Brayton Cycle

The basic Brayton cycle comprises four processes, namely isentropic compression, isobaric heat addition, isentropic expansion, and isobaric heat rejection. The mechanical devices that perform these processes are the compressor, heater, turbine, and cooler, indicated schematically in the plant diagram of Fig. 7.7. The fact that in Brayton cycle the heat addition and rejection processes are isobaric rather than isothermal means that this cycle is externally irreversible.

Due to the direct connection with the atmosphere, the intake pressure and gas expelling pressure are equal to the atmospheric pressure which represents a limitation of turbine's working conditions. This limitation can be overcome if the cycle is closed using a heat exchanger having the role of a cooler. Henceforth, the turbine can be made to discharge in vacuum which means that more work is generated and an enhanced efficiency is obtained. The turbine discharge pressure can be adjusted indirectly by varying the heat sink temperature.

Combustion turbine power cycles started to develop commercially in 1930s based on simple Brayton cycle of open type which includes a turbo compressor, a combustion chamber, and gas turbine. A large pallet of fuels can be used for Brayton cycle, starting with natural gas, fuel oil, coal gas, etc. The efficiency of combustion turbine power plants reach remarkable values of over 40 % in conditions when the expelled gases are still at elevated temperature (over 625 K).

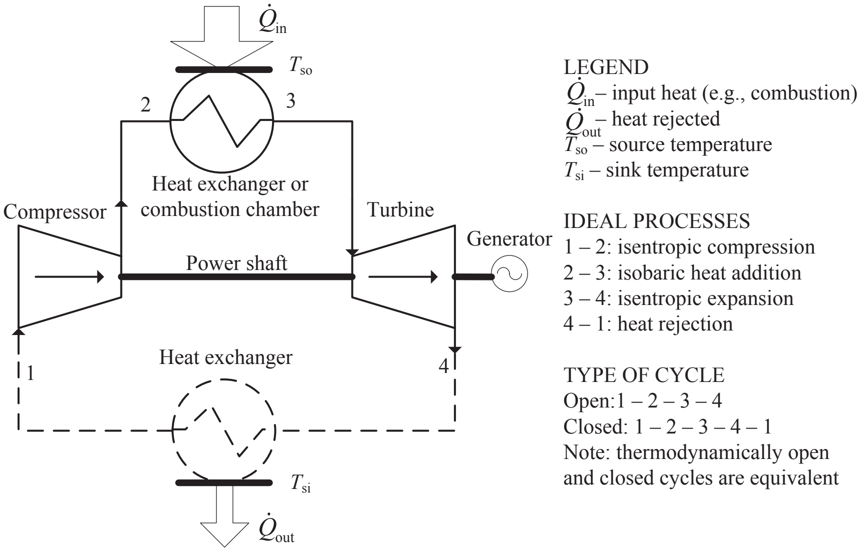

Fig. 7.7 Schematic of a simple Brayton cycle-based power plant

In an actual combustion turbine, the working fluid is represented by pressurized combustion gases which expand and generate power. In order to make fuel utilization efficient, the excess air provided to combustion chamber can be in the range of minimum 4 up to over 50. Henceforth, air is well present in combustion gases, and consequently, approximating the properties of combustion gases with that of air is generally accepted. When the working fluid is modeled as ideal gas air with specific heat corresponding to 298 K ($c_p = 1.005$ kJ/kgK, $\gamma = 1.4$), then the cycle is denoted as “air-standard Brayton cycle.” If all internal processes are reversible, then the cycle is called “ideal air-standard Brayton cycle.”

Closed Brayton cycle (1–2–3–4–1 in the figure) must operate with an inert working fluid, either dry air or helium. The heat input can be derived from a combustion process but is applied externally—by heat transfer—to the heater process 2–3. The combustion gases never mix with the working fluid in this case, and the Brayton cycle-based system becomes a so-called external combustion engine. It is important to note that the open and close Brayton cycles are equivalent from thermodynamic point of view.

The *T–s* diagram of an ideal air-standard Brayton cycle of basic configuration is shown in Fig. 7.8. For the air-standard Brayton cycle, perfect gas equation of state can be applied to further derive analytical expressions for cycle efficiency. The perfect gas is the ideal gas with constant specific heats (independent of temperature). As mentioned above, for standard air, the specific heats are estimated for 298.15 K. Using the general equation $\Delta h = C_p \Delta T$ and the EBE, the energy efficiency becomes

$$\eta = 1 - \frac{C_p\left(T_4 - T_1\right)}{C_p\left(T_3 - T_2\right)} = 1 - \left(\frac{T_1}{T_2}\right)\frac{\left(\frac{T_4}{T_1}\right) - 1}{\left(\frac{T_3}{T_2}\right) - 1}$$

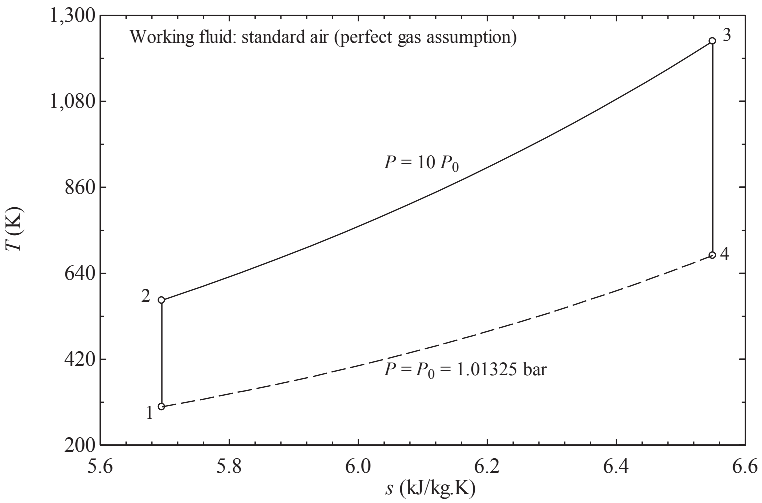

Fig. 7.8 Representation of a basic air-standard Brayton cycle in *T*–*s* diagram for $r = 10$ and $T_1 / T_3 = 0.24$

Another general equation for perfect gas describes the interrelation between pressure and temperature along an isentropic process 1–2 according to $T_1 P_2^\kappa = T_2 P_1^\kappa$, with

$$\kappa = (\gamma - 1)/\gamma$$

and γ the specific heat ratio. Since processes 1–2 and 3–4 are isentropic and evolve between the same pressures, $P_1 = P_4$ and $P_3 = P_2$, one has

$$\frac{T_3}{T_4} = \left(\frac{P_3}{P_4}\right)^\kappa = \left(\frac{P_2}{P_1}\right)^\kappa = \frac{T_2}{T_1} \rightarrow \frac{T_4}{T_1} = \frac{T_3}{T_2}.$$

Therefore, the energy efficiency of air-standard Brayton cycle becomes

$$\eta = 1 - r^{-\kappa}, \quad \text{with pressure ratio defined by } r = \frac{P_2}{P_1} > 1 \tag{7.21}$$

7.4 Energy and Exergy Analyses of Locomotive Systems

The locomotive prime mover is generally powered by a large two-stroke compression ignition (CI) diesel-fueled engine. Modern diesel CI engine cycles operate between upper and lower limits of the Otto and Diesel cycles according to the thermodynamic dual cycle discussed above. When modeling the CI engine for the locomotive, its actual parameters including size, power generation magnitude, and mass flow rates of involved flows must be considered. The ideal gas behavior assumption is in general considered valid.

The mass flow of air ($\dot{m}_a$) drawn into the intake manifold is determined based on engine geometry and rated operating conditions, for air composed of 21 % oxygen and 79 % nitrogen (which means that 3.76 mol or kmole of nitrogen for 1 mol or kmole of oxygen is required for a stoichiometric combustion), by the following equation:

$$\dot{m}_a = \eta_v \left[\frac{P_{im} \cdot V_D \cdot N_{ICE} \cdot (0.21 M_{O2} + 0.79 M_{N2})}{R_u \cdot T_{im}} \right] \tag{7.22}$$

where T_{im} and P_{im} are the temperature and pressure after the turbocharger, V_D is the total volume displacement of the combustion engine, N_{ICE} is the rated engine speed which is converted to rev/s units, and the volumetric efficiency, η_v, is assumed here to be 0.95.

Energy efficiency for the locomotive compression ignition engine is defined as the ratio of the useful power produced at rated conditions to the energy input. We denote by $\dot{W}_{TP}$ the locomotive traction power, and by $\dot{Q}_{in}$ the thermal energy supplied by fuel. Thus, one has

$$\eta_{ICE} = \frac{\dot{W}_{TP}}{\dot{Q}_{in}} \tag{7.23}$$

For the mixed fueling case, $\dot{Q}_{in}$ is the sum of the energy input for each fuel, calculated from the mass flow rate and lower heating value of each fuel according to:

$$\dot{Q}_{in} = \eta_c \cdot \sum (\dot{m}_f \cdot LHV_f) \tag{7.24}$$

where combustion is assumed to be complete ($\eta_c = 1.0$) for the general case.

Exergy efficiency of the ICE is similarly defined as the ratio of useful power to the exergy content of the fuel input, given by

$$\psi_{ICE} = \frac{\dot{W}_{TP}}{\dot{E}x_{in}} \tag{7.25}$$

where the exergy of the fuel input is given by $\dot{E}x_{in} = \sum \left[\dot{m}_i \cdot (ex_{ph} + ex_{ch})_i \right]$, and ex_{ph} and ex_{ch} are the physical and chemical exergy values of the supplied fuel(s).

It is useful to define the overall energy and exergy balances for the engine in terms of heat and work duties and losses, since a portion of the heat energy losses from the engine represent potential performance gains if applied as process heating in the integrated ammonia systems. Engine cooling requirement is met by the water jacket cooling ($\dot{Q}_{wjc}$) and aftercooler ($\dot{Q}_{ac}$) systems, where cooling loads are related to the locomotive traction power by the equations:

$$\dot{Q}_{\mathrm{wjc}} = HRR_{\mathrm{wjc}} \cdot \dot{W}_{\mathrm{TP}} \tag{7.26}$$

$$\dot{Q}_{\mathrm{ac}} = HRR_{\mathrm{ac}} \cdot \dot{W}_{\mathrm{TP}} \tag{7.27}$$

where HRR_{i} terms refer to heat removal rates by the aftercooler and water jacket of the engine.

For the locomotive engine, the heat removal rate is approximately 1.19 kW for the kW of traction power. The total heat removed for engine cooling is the sum of these, $\dot{Q}_{\mathrm{ec}} = \dot{Q}_{\mathrm{wjc}} + \dot{Q}_{\mathrm{ac}}$. The associated thermal exergy rate is evaluated using the general equation for exergy of heat, according to the following equation:

$$\dot{E}x_{\mathrm{j}}^{\mathrm{Q}} = \left(1 - \frac{T_{\mathrm{o}}}{T_{\mathrm{j}}}\right)\dot{Q}_{\mathrm{j}} \tag{7.28}$$

The energy and exergy balances for the internal combustion engine are the totals of the work and heat rates, and the system losses produced by the fuel energy supplied are defined by the equations:

$$\dot{Q}_{\mathrm{in}} = \sum(\dot{m} \cdot h)_{\mathrm{exh}} - \sum(\dot{m} \cdot h)_{\mathrm{a}} + \dot{W}_{\mathrm{TP}} + \dot{W}_{\mathrm{acc}} + \dot{Q}_{\mathrm{rec}} + \dot{Q}_{(\mathrm{ac+wjc})} \tag{7.29}$$

$$\begin{aligned} \dot{E}x_{\mathrm{in}} = {} & \sum(\dot{m} \cdot ex)_{\mathrm{exh}} - \sum(\dot{m} \cdot ex)_{\mathrm{a}} + \dot{W}_{\mathrm{TP}} \\ & + \dot{W}_{\mathrm{acc}} + \dot{E}x_{\mathrm{rec}}^{Q} + \dot{E}x_{(\mathrm{ac+wjc})}^{Q} + \dot{E}x_{\mathrm{loss}} + \dot{E}x_{\mathrm{d}} \end{aligned} \tag{7.30}$$

where accessory work, $\dot{W}_{\mathrm{acc}}$, represents the power required for cooling and lubrication systems, and the energy loss term, $\dot{E}_{\mathrm{loss}}$, represents heat loss due to friction, mixing heat transfer, and electromechanical losses associated with the conversion of shaft power to electricity, assuming generator conversion efficiency, η_{gen}, of 0.95.

Exergy destruction, $\dot{E}x_{\mathrm{d}}$, is the loss from the engine that is not recovered. The individual losses, $\dot{E}x_{\mathrm{d,i}}$, include internal and external destructions, where the internal losses are irreversible, and a portion of the external losses may be recovered (i.e., exhaust gases at high temperature). The primary sources of exergy destruction are compared using the exergy destruction ratio given by

$$ExDR = \frac{\dot{E}x_{\mathrm{d,i}}}{\dot{E}x_{\mathrm{d,TOT}}} \tag{7.31}$$

The major components applied throughout the engine locomotive systems processes include compressors, turbines, heat exchangers, and pumps. The balance equations, including mass, energy, entropy, and exergy balances for these components are given in Table 7.2, based on the inlet and exit streams and the input and output

Table 7.2 Mass, energy, entropy, and exergy balance equations of common components

Component	Balance equations[a]	Component efficiency
Compressor	$\dot{m}_{\mathrm{i}} = \dot{m}_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} h_{\mathrm{i}} + \dot{W}_{\mathrm{j}} = \dot{m}_{\mathrm{e}} h_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} s_{\mathrm{i}} + \dot{S}_{\mathrm{gen,\,j}} = \dot{m}_{\mathrm{e}} s_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} ex_{\mathrm{i}} + \dot{W}_{\mathrm{j}} = \dot{m}_{\mathrm{e}} ex_{\mathrm{e}} + \dot{E}X_{\mathrm{d,j}}$	$\eta_{\mathrm{C,s}} = \left(h_{\mathrm{e,\,s}} - h_{\mathrm{i}}\right) / \left(h_{\mathrm{e}} - h_{\mathrm{i}}\right)$ $h_{\mathrm{e,\,s}} = h\left(P_{\mathrm{e}}, s_{\mathrm{i}}\right)$
Turbine	$\dot{m}_{\mathrm{i}} = \dot{m}_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} h_{\mathrm{i}} = \dot{m}_{\mathrm{e}} h_{\mathrm{e}} + \dot{W}_{\mathrm{j}}$ $\dot{m}_{\mathrm{i}} s_{\mathrm{i}} + \dot{S}_{\mathrm{gen,j}} = \dot{m}_{\mathrm{e}} s_{\mathrm{e}}$ $\mid \dot{m}_{\mathrm{i}} ex_{\mathrm{i}} = \dot{m}_{\mathrm{e}} ex_{\mathrm{e}} + \dot{W}_{\mathrm{j}} + Ex_{\mathrm{d,j}}$	$\eta_{\mathrm{T,\,s}} = \left(h_{\mathrm{i}} - h_{\mathrm{e}}\right) / \left(h_{\mathrm{i}} - h_{\mathrm{e,\,s}}\right)$ $h_{\mathrm{e,\,s}} = h\left(P_{\mathrm{e}}, s_{\mathrm{i}}\right)$
Pump	$\dot{m}_{\mathrm{i}} = \dot{m}_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} h_{\mathrm{i}} + \dot{W}_{\mathrm{j}} = \dot{m}_{\mathrm{e}} h_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} s_{\mathrm{i}} + \dot{S}_{\mathrm{gen,j}} = \dot{m}_{\mathrm{e}} s_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} ex_{\mathrm{i}} + \dot{W}_{\mathrm{j}} = \dot{m}_{\mathrm{e}} ex_{\mathrm{e}} + \dot{E}x_{\mathrm{d,j}}$	$\eta_{\mathrm{P,\,s}} = \left(h_{\mathrm{e,\,s}} - h_{\mathrm{i}}\right) / \left(h_{\mathrm{e}} - h_{\mathrm{i}}\right)$ $h_{\mathrm{e,\,s}} = h\left(P_{\mathrm{e}}, s_{\mathrm{i}}\right)$
Heat exchanger	$\sum \dot{m}_{\mathrm{i}} = \sum \dot{m}_{\mathrm{e}}$ $\sum \dot{m}_{\mathrm{i}} h_{\mathrm{i}} = \sum \dot{m}_{\mathrm{e}} h_{\mathrm{e}} + \Delta \dot{Q}_{\mathrm{j}}$ $\sum \dot{m}_{\mathrm{i}} s_{\mathrm{i}} + \dot{S}_{\mathrm{gen,\,j}} = \sum \dot{m}_{\mathrm{e}} s_{\mathrm{e}} + \dfrac{\Delta \dot{Q}_{\mathrm{j}}}{T_{\mathrm{o}}}$ $\sum \dot{m}_{\mathrm{i}} ex_{\mathrm{i}} = \sum \dot{m}_{\mathrm{e}} ex_{\mathrm{e}} + \dot{E}x_{\mathrm{j}}^{\mathrm{Q}} + \dot{E}x_{\mathrm{d,j}}$	$\varepsilon_{\mathrm{HX}} = \dot{Q}_{\mathrm{useful}} / \dot{Q}_{\mathrm{max}}$ $\dot{Q}_{\mathrm{max}} = (\dot{m}_{\mathrm{i}} c_{\mathrm{p,\,i}})_{\mathrm{min}} \cdot (T_{\mathrm{max}} - T_{\mathrm{min}})$
Expansion valve	$\dot{m}_{\mathrm{i}} = \dot{m}_{\mathrm{e}}$ $h_{\mathrm{i}} = h_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} s_{\mathrm{i}} + \dot{S}_{\mathrm{gen,j}} = \dot{m}_{\mathrm{e}} s_{\mathrm{e}}$ $\dot{m}_{\mathrm{i}} ex_{\mathrm{i}} = \dot{m}_{\mathrm{e}} ex_{\mathrm{e}} + \dot{E}x_{\mathrm{d,j}}$	–

[a] Balance equations refer to inlet (i) and exit (e) streams of j-component

power and heat fluxes. The component efficiency is given in terms of the isentropic efficiency of work input/output components, and effectiveness of heat exchange processes.

To compare the performance of the locomotive engine systems to a baseline locomotive performance, it is necessary to quantify performance gains from any possible additional work and heat recovery processes. Utilization efficiencies (η_{u}) are defined for the system(s) using the following general equation:

$$\eta_{\mathrm{u}} = \frac{\dot{W}_{\mathrm{TP}} + \dot{W}_{\mathrm{net}} + \dot{Q}_{\mathrm{ref}} + \sum \dot{Q}_{\mathrm{useful}}}{\dot{Q}_{\mathrm{in}}} \tag{7.32}$$

where the net work, $\dot{W}_{\mathrm{net}}$, includes the additional work produced/consumed by the system components (turbines, pumps, and compressors), and $\dot{Q}_{\mathrm{ref}}$ is the heat rate consumed by the fuel reformation systems which applies when the engine system include such process.

The general equation for the exergetic utilization efficiency of the systems is essentially defined as

$$\psi_{\mathrm{u}} = \frac{\dot{W}_{\mathrm{TP}} + \dot{W}_{\mathrm{net}} + \left(1 - \frac{T_{\mathrm{o}}}{T_{\mathrm{DSU}}}\right) \cdot \dot{Q}_{\mathrm{ref}} + \sum \dot{E}^{Q}_{\mathrm{useful}}}{\dot{E}x_{\mathrm{in}}}. \tag{7.33}$$

For integrated cooling systems that require work input, a coefficient of performance ($\mathrm{COP_c}$) is applied to simplify the calculation of the required work input ($\dot{W}_{\mathrm{in}}$), given by

$$\left|\mathrm{COP_c}\right| = \left|\frac{\dot{Q}_{\mathrm{c}}}{\dot{W}_{\mathrm{in}}}\right| \tag{7.34}$$

where $\dot{W}_{\mathrm{in}}$ represents pump and/or compressor duties to power cooling systems.

When considering exergy in environmental impact analysis, the inventory analysis phase has to account more carefully for mass and energy flows into, out of, and through all the stages of the life cycle; next, the energy flow is associated with an exergy flow; eventually, environmental impact indicators based on exergy can be developed and studied.

7.5 Environmental Impact Assessment

In recent years, particular emphasis has been placed on releases of carbon dioxide, since it is the main greenhouse gas (GHG), and optimization of thermal systems based on this parameter has received much attention. A focus of many studies is to consider emissions of the following types of atmospheric pollutants: CO, NO_x, SO_2, CO_2, and CH_4. In the case of railway transportation which is fueled by a combustion process, the atmospheric pollution through flue gas emissions is very relevant.

Many statistical data and analyses are available in the literature for the conventional locomotive systems. Regarding the projected, low-emission locomotive systems and fuel, there is a lack of such data in the literature, explained by the fact that the newer system has not been built yet at large scale; only small prototype, laboratory tests, and theoretical analyses are available for those.

An assessment of the environmental impact of a locomotive system requires the analysis and modeling of the combustion gas emission process. Besides biofuels, natural gas, methanol, ammonia, and hydrogen are the main replacement fuels for clean-air transportation. Combustion properties of the fuels are key information for any emission modeling. Here, in Table 7.3, we present the main properties of selected fuels considered in the case studies that are presented at the end of this book; the fuels are ammonia and hydrogen, whereas the ultra-low sulfur diesel (ULSD) is taken as a baseline case (Table 7.4).

The stoichiometric reaction equations are given in Table 7.5 for each fuel. For fuel blends NH_3-ULSD and NH_3-ULSD-H_2, the equations are combined based on the fraction of fuel energy provided by NH_3 to maintain the required energy

Table 7.3 Combustion properties of NH_3, ULSD, and H_2 fuels

Specification	Ammonia	ULSD	Hydrogen
Molecular formula	NH_3	$C_{12}H_{23}$	H_2
Molecular weight, M_i (kg/kmol)	17.03	167.3	2.016
Stoichiometric air–fuel ratio (molar), a_{st} ($kmol_{air}/kmol_i$)	0.75	17.75	0.5
Stoichiometric air–fuel ratio (mass), AF_{st} (kg_{air}/kg_i)	6.05	14.57	34.2
Stoichiometric energy content (MJ/kg_{mix})	3.4	2.77	2.64
Ignition limits (%-vol. in air)	16–25	0.6–5.5	4–75
Adiabatic flame temperature (°C)	1850	1977	2000
Autoignition temperature (°C)	651	~225	571

ULSD ultra-low sulfur diesel

Table 7.4 Stoichiometric combustion reactions

Fuel	Molecular formula	Combustion reaction
ULSD	$C_{12}H_{23}$	$C_{12}H_{23}+17.75\cdot(O_2+3.76\cdot N_2)\rightarrow 12\cdot CO_2+11.5\cdot H_2O+17.75\cdot(3.76)\cdot N_2$
Ammonia	NH_3	$NH_3+0.75\cdot(O_2+3.76\cdot N_2)\rightarrow 1.5\cdot H_2O+3.32\cdot N_2$
Hydrogen	H_2	$H_2+0.5\cdot(O_2+3.76\cdot N_2)\rightarrow H_2O+0.5\cdot(3.76)\cdot N_2$

Table 7.5 Fuel emission factors and global warming potential of GHGs for ULSD. (Source: Ref. [20])

Gas species	Emission factor, EF_i (kg/L)	Global warming potential, GWP_i
Carbon dioxide (CO_2)	2.66300	1
Methane (CH_4)	0.00015	21
Nitrous oxide (N_2O)	0.00110	310
Carbon dioxide equivalent $CO_{2\ eq}$.	3.00715[a]	–

[a] Emission factor, $EF_{CO_2\ eq}.=\Sigma(EF_i\cdot GWP_i)$

Table 7.6 Fuel- and feedstock-related GHG emissions (kg $CO_{2,\ eq}$/L). ((Source: Ref. [45]))

Fuel	NH_3	ULSD
Feedstock	Natural gas	Crude oil
Production/feedstock	1.0831	0.4227
Fuel combustion	0	2.668
TOTAL	1.0831	3.0908

based on LHV. The emission data for ULSD are given in Table 7.5. When a fuel blend using ULSD is analyzed, then this emission data can be used to determine the proportion of GHG emissions due to the diesel fuel component. The fuel- and feedstock-related GHG emissions are both taken into account. Table 7.6 gives the feedstock-related GHG emissions for ammonia and ULSD.

Table 7.7 Conventional diesel locomotive emission factors (ULSD). (Source: Ref. [20])

Emission type	Emission factor, EF_i (kg/L)	
	Passenger	Freight
Particulate matter (PM)	0.00118	0.00123
Hydrocarbon(s) (HC)	0.00223	0.00238
Nitrogen oxides (NO_x)	0.05623	0.04923
Carbon monoxide (CO)	0.00703	0.00706

Table 7.8 Compact SCR™ locomotive emission reduction (g/BHP hr). (Source: Ref. [98])

Duty cycle	Standard	HC (%)	NO_x (%)	PM (%)	CO (%)
Line-haul	Compact SCR™ reduction	>90	71	61	82
Switch	Compact SCR™ reduction	>90	61	57	93

Emission factors for conventional locomotives are considered as given in Table 7.7. These factors allow for the correlation of ULSD emissions with the fuel consumption. However, the sulfur dioxide (SO_2) emissions can be determined from the sulfur content of diesel fuel by the following equation:

$$EF_{SO_2} = 10^{-6} \rho_{ULSD} \cdot \left(\frac{M_{SO_2}}{M_S} \right) \cdot S_{ppm} f_{c,SO_2} \tag{7.35}$$

where f_{c,SO_2} represents a conversion factor (S→SO_2). Note that from Eq. (7.35), for ULSD containing 15-ppm sulfur, liquid density $\rho_{ULSD} = 850$ kg/m^2, and an assumed conversion factor of $f_{c,SO_2} = 0.98$ (S→SO_2), the resulting emission factor is $EF_{SO_2} = 0.025 \text{g} / \text{L}$.

Regarding the NO_x emission reduction by the selective catalytic reduction (SCR) unit, this can be modeled based on manufacturer data for SCRs installed in an operational locomotives. Such data are given in Table 7.8 for the EMD 12-710G3 diesel engine as provided by the manufacturer, namely in terms of percent reduction from baseline locomotive operation without SCR installed.

These reductions are applied to diesel combustion emissions, which are determined using current Tier 2 emission standards to indicate the improvement potential of utilizing SCR in locomotives in baseline operation. The mass flow rate of NO_x is correlated with the fraction of ULSD consumed, and the NO_x emission factors for emission limits are given in Table 7.7.

Regarding the emission analysis from ammonia or ammonia–diesel combustion when applied, it can be assumed that the molar ratio of supplied NH_3 to NO_x is 1:1, according to the main reaction as follows:

$$4NH_3 + 4NO + 4O_2 \rightarrow 6H_2O + 4N_2 \tag{7.36}$$

Ammonia combustion may be assumed to be complete provided that sufficient oxidant is provided. However, for the practical case where some NO_x results in the NH_3

combustion reaction, emissions may be easily controlled by adjusting the supply of NH_3 to the SCR, while also taking care to ensure that NH_3 slip does not exceed the Environmental Protection Agency (EPA) limit of 2–10 ppm NH_3 in the exhaust stream.

Also, the NO_x and carbon monoxide emissions for hydrocarbon fuels can be correlated with the adiabatic flame temperature and the combustion pressure. Some simplified models can be used as an alternative for such cases as presented elsewhere [102], which relate the mass flow rate of CO and NO_x emissions with the fuel (natural gas) consumption

$$\frac{\dot{m}_{\mathrm{CO}}}{\dot{m}_{\mathrm{f}}} = 179{,}000 \frac{\exp\left(\frac{7800}{T}\right)}{P^2 \tau \left(\frac{\Delta P}{P}\right)^{0.5}} \tag{7.37}$$

$$\frac{\dot{m}_{\mathrm{NOx}}}{\dot{m}_{\mathrm{f}}} = 150{,}000 \frac{\tau^{0.5} \exp\left(-\frac{71{,}100}{T}\right)}{P^{0.05} \tau \left(\frac{\Delta P}{P}\right)^{0.5}} \tag{7.38}$$

where T is the adiabatic flame temperature, P is combustion pressure, ΔP is the pressure drop across the combustion chamber, and τ is the residence time in the combustion zone (approximately 2 ms).

Hydrogen produced by thermo-catalytic decomposition of ammonia in the decomposition and separation unit (DSU) is used as a combustion fuel to further reduce the diesel fuel consumption and to assist the combustion of ammonia in the ICE. The decomposition occurs according to the reaction:

$$NH_3 \xrightarrow{\Delta h_d} \frac{3}{2} H_2 + \frac{1}{2} N_2$$

where the heat of the endothermic reaction, Δh_d, is determined as a function of temperature [8]. The decomposition may be written based on the dissociation fraction, x_d, describing the amount of each gas species in the product gas mixture by

$$NH_3 \rightarrow \frac{3x_d}{2} H_2 + \frac{x_d}{2} N_2 + (1 - x_d) NH_3. \tag{7.39}$$

The heat required for the reaction is given in terms of the enthalpy change of ammonia to raise its temperature to the required level for decomposition, and the extent of the dissociation, given by

$$\Delta h_{\mathrm{DSU}}(T) = h_o(T) - h(T_o) + x_d \cdot \eta_d \cdot \Delta h_d(T) \tag{7.40}$$

Table 7.9 Main characteristics of the ammonia decomposition process

Chemical reaction equation	$NH_3 \rightarrow 1/2\ N_2 + 3/2\ H_2$
Standard enthalpy of reaction, ΔH_{NH3} (kJ/mol)	45.90
Operating temperature, T_{DSU} (°C)	350–525

where the efficiency of the decomposition process, η_d, is assumed to be 0.9 [8].

General operating characteristics for a decomposition unit are given in Table 7.9. To obtain the temperature necessary for the DSU reaction in the proposed systems, a portion of the exhaust stream is used to heat the ammonia to a temperature within the given range. The further integration of the NH_3 supply and N_2 product streams within the propulsion systems, such as engine cooling (heat recovery) and expansion work, are described in the technology by [77], and applied to the various locomotive engine systems.

There are two major system frameworks to consider when assessing the overall sustainability of a railway locomotive—the prime mover and the fuel. These frameworks are depicted in Fig. 7.9, indicating the major drivers affecting the performance of each system. While these frameworks may each be addressed separately, they are ultimately linked since the sustainability of locomotive operation is affected by both the propulsion system efficiency and the fuel/energy resource sustainability in terms of generated GHG and other emissions.

Impact factors are used to evaluate the results of the energy, exergy, environmental, and economic analyses, and assess the performance of the proposed systems in terms of overall sustainability and feasibility. These factors provide a method for performance comparison from various perspectives in order to make objective recommendations for system selection.

The environmental impact of alternative fueling on GHG emissions produced in fuel combustion is described by a greenization factor (GF), which indicates the degree of CO_2 reduction, given by

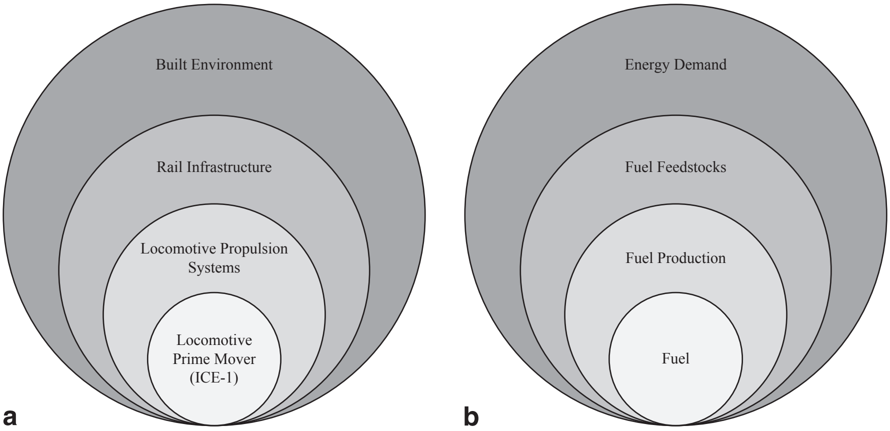

Fig. 7.9 Framework for sustainable locomotive: **a** prime mover aspects and **b** fuel aspects

$$\mathrm{GF} = \frac{\dot{m}_{\mathrm{CO_2,ref}} - \dot{m}_{\mathrm{CO_2,Sys_i}}}{\dot{m}_{\mathrm{CO_2,ref}}}, \tag{7.41}$$

where the reference case is that of diesel-only combustion.

The environmental impact analysis must account for the impact of the system effluents to the environment and also the pollution and resource depletion related to the system and its components' construction and maintenance. In this context, considering exergy as a tool for the environmental impact analysis is beneficial. The inventory analysis phase has to account more carefully for mass and energy flows into, out of, and through all the stages of the life cycle. The energy flow is associated with an exergy flow. Eventually, environmental impact indicators based on exergy can be developed and studied.

The inventory analysis is the core of the environmental impact analysis as it determines the streams of materials and their impact on the environment. All flows of matter exchanged with the environment, and their interrelationship within the analyzed system must be inventoried. For conducting an exergoenvironmental analysis, the system itself is modeled in an expanded form, by including two additional systems: upstream—the system construction process, and downstream—effluent environmental and decommissioning processes. Therefore, the total exergy supply to be considered in an extended exergoenvironmental analysis is

$$\dot{E}x_{\mathrm{supply}} = \dot{E}x_{\mathrm{direct}} + \dot{E}x_{\mathrm{indirect}}^{\mathrm{upstream}} + \dot{E}x_{\mathrm{indirect}}^{\mathrm{downstream}}. \tag{7.42}$$

A similar equation can be also written for the environmental impact, namely

$$EI_{\mathrm{total}} = EI_{\mathrm{direct}} + EI_{\mathrm{indirect}}. \tag{7.43}$$

where EI is a general environmental impact indicator, EI_{direct} represents the downstream environmental impact, that is, the environmental impact caused by the system due to its operation, and EI_{indirect} represents the environmental impact associated with system construction.

A primary objective of exergoenvironmental analysis is the identification and quantification of direct and/or indirect environmental impact in correlation with exergy destroyed by the system. Another objective is to minimize the environmental impact. Often this is done by finding means of increasing the energy efficiency of the system. Another approach to environmental impact minimization is the reduction of the polluting effluents.

7.6 Economic Assessment

Economics is crucial in guiding the engineering decisions in implementation of various sustainable energy systems and technologies. Politics, of course, influences the economic decision toward sustainable practices. A key aspect of the clean-rail economics is related to the emission tax enforcements and other legislation, regulations, standards, and codes. These costs may include carbon tax, tax deductions on clean air, incentives, and bonds which are given by governments to help initial investments in greener technologies.

Aspects as such can change the economic picture in general and accelerate the march of societies toward a globally spread sustainable energy practice. Many jurisdictions rely nowadays on various financial incentives that modify the life cycle cost or saving such that sustainable energy sources are promoted by making them economically attractive. Examples of these policy/economic measures are as follows:

- Exemption from taxes
- Capital grants
- Auction to supply contracts for renewable energy
- Financial obligations or bonds on promoting clean air initiatives
- "Fill-in" tariffs (i.e., fixed premium prices for clean fuels and electricity)

One major item in economic analysis is the capital cost. Its fair estimation depends on various economic factors and fluctuating prices. However, some guidelines for cost estimation of main process equipment in the industry do exist. The costing equations for the main equipment involved in railway locomotive systems are given in Table 7.10.

Although there may be some variations in the economic engineering analysis of the system, here we describe a simple approach which leads to the determination of the discounted capital in present worth and does not consider loans, but only invested capital. The economic analysis requires first to establish a set of parameters as given in Table 7.11. The main equations for an economic analysis are given in Table 7.12. The most basic notion in economics is probably the *capital* that refers to items of extensive value. Even though the term capital has several other significances, we refer here only to *financial capital* which represents a value owned by legal entities that can be saved, traded, and can be predictably useful when retrieved.

When traded, the financial capital can be liquidated as *money*, because by their nature money are used as medium of exchange. It is important to remark that market value of a capital is not based on the historical accumulation of money invested but on the perception by the market of its expected revenues and of the risks entailed. The revenue may come from the investment of financial capital in the form of money. Since money can be invested, they augment the capital and thus the future worth of money always increases. Said in the other way around, the present worth of money (or of a capital measured by money) is always smaller than the future worth.

One says that the present worth is discounted with respect to the future worth. By definition, the *rate of discounting the future* (or the discount rate) represents the incremental growth of worth during a period of time. Application of the discount rate for more than one period is known as *compounding*. Through compounding, one obtains the ratio between the future and present worth. The present and future worth are general notions because they refer to values. For example, they apply to money that increases their present value due to the productivity of capital, but these

Table 7.10 Cost on relevant equipment (given in 1981 US\$). [103–105]

Equipment type	Costing equation
Centrifugal compressors without drivers	$C[\text{k\$}] = 6.49\left(\dot{W}[\text{HP}]\right)^{0.62}$
Reciprocating compressors without drivers	$C[\text{k\$}] = 5.96\left(\dot{W}[\text{HP}]\right)^{0.61}$
Fans with backward curved blades, with drivers	$C[\text{k\$}] = f_\text{m} f_\text{p} \exp\left(0.04 + 0.1821\ \ln(\dot{V}) + 0.0786\ \ln^2(\dot{V}^2)\right)$, where f_m is blade material factor; f_p is pressure factor; $f_\text{m} = 2.2$ (carbon steel), 5.5 (fiber glass, 4.0 (fiberglass), 11.0 (nickel alloy); $f_\text{p} = 1.0$ for $\Delta P < 1$ kP, 1.3 for $\Delta P < 8$ kPa; $\dot{V}$ is the flow rate in thousands of SCFM
Turbines	$C[\text{k\$}_{1981}] = 0.31\left(\dot{W}[\text{HP}]\right)^{0.81}$
Long tube evaporators	$C[\$] = f_\text{m}\left(A[\text{sqft}]\right)^{0.85}$; f_m is material factor $f_\text{m} = 1.0$ (carbon steel/copper), 0.6 (steel/steel), 0.7 (steel/aluminum), 3.3 (nickel/nickel); A is the heat transfer area
Shell and tube heat exchangers	$C[\$] = 1.35 f_\text{m} f_\text{p} \exp\left(8.821 + 0.0681 \ln(A) + 0.0786 \ln^2(A^2)\right)$, where f_m is material factor; f_p is pressure factor; $f_\text{m} = c_1 + c_2 \ln A\, f_\text{p} = 1.03 + 0.07 \ln A$; $c_1 = 0.8$ (stainless steel), 1.5 (nickel), 1.3 (monel), 1.2 (inconel), 1.5 (titanium), 0.15 (hastelloy); $c_2 = 0.2$ (stainless steel), 0.5 (nickel), 0.4 (monel), 0.5 (inconel), 0.4 (titanium), 0.5 (hastelloy); A is the heat transfer area in sqft
Electric motors at 3600 RPM	$C[\$] = 1.2 \exp\left(4.8 + 0.097 \ln(\dot{W}) + 0.1 \ln^2(\dot{W}^2)\right)$ for $\dot{W} < 7.5\text{HP}$ $C[\$] = 1.2 \exp\left(4.1 + 0.5 \ln(\dot{W}) + 0.05 \ln^2(\dot{W}^2)\right)$ for $\dot{W} < 250\text{HP}$ $C[\$] = 1.2 \exp\left(4.3 + \ln(\dot{W}) 0.03 \ln^2(\dot{W}^2)\right)$ for $\dot{W} < 700\text{HP}$
Reciprocating pumps without motor	$C[\text{k\$}] = 40\dot{V}^{0.81}$ for cast iron material and $\dot{V} < 400\text{gpm}$ $[\text{k\$}] = 410 f_\text{m} \dot{V}^{0.52}$ for $\dot{V} < 400$ gpm and the material factor $f_\text{m} = 1$ (stainless steel), 1.4 (brass), 1.86 (aluminum), 2.2 (monel)

concepts also apply to any commodity. It is interesting to remark that the taxes increase in time at constant rate.

Another aspect regarding the discount rate is brought by the volatile nature of money that has the quality to inflate or deflate. Inflation refers to increase over the time of the average *price* of goods and services. Through the term price we understand the assignment of a monetary value to a good or service. Any price is given in a specific currency that represents a unit of trade which is a measure of money.

Deflation is the opposite of inflation, representing decrease over the time of the average purchasing power of money. Both inflation and deflation phenomena come in succession, that is, after a period of inflation may come a period of deflation depending on the march of the economy as whole. They can be quantified by accounting on the relative variation of currency.

The rate of discount of any kind of business is affected by inflation and deflation because these modify the cash flows associated with any economic (and engineering) project conducted over a time period. Therefore, it is important to quantify these effects and their impact on the discount rate. Inflation and deflation can be

Table 7.11 Parameters required for an economic analysis

Parameter	Symbol	Description
System lifetime	n	Number of years (or discount periods) of the system under investigation
Real discount rate	r	Rate of return for the discounted cash flow to determine value
Inflation rate	i	This is a sub-unitary factor accounting for inflation rate
Renewable energy (incl. biofuels) tax credit	t_c	When renewable energy (incl. biofuels) is used, a tax credit may apply, $t_c \in [0,1)$
Tax on income	t_i	Tax applied in any income of money coming from output costs, $t_i \in [0,1)$
Tax on property	t_p	Tax applied to the property value, $t_p \in [0,1)$
Tax on salvage	t_s	Tax applied on the salvage value of the system, $t_s \in [0,1)$
Capital salvage factor	CSF	At the end of lifetime, a fraction *CSF* of the invested capital is recovered
Levelized product (travel) price	LPP	The price in dollar with which the unit of product is sold (in present worth). Here, the levelized travel price can be used
Annual production	AP	Number of units of product for one year (or one discount period)
Levelized cost of consumables	LCC	The sum of all input costs (fuels, supplies) levelized for present worth
Annual consumption	AC	The annual consumption of consumables
Operation and maintenance cost factor	$OMCF$	A sub-unitary fraction of either the net income or the invested capital
Invested capital	$\mathcal{C}_{\mathrm{cap}}$	A monetary value (in \$) paid upfront (in equity) to initiate the business

quantified through the *consumer price index* (CPI) that represents the average price of a "basket" of goods in a given period, divided by the price of the same basket in a base period. Since it refers to price, the CPI is always given with respect to a specific currency.

The CPI provides a mean to differentiate among the real worth and nominal worth of a currency. The *real worth of a currency* (RW) represents the worth of that currency in the reference period taken by convention, for computing the CPI. The *nominal worth of currency* (NW) refers the actual worth at the current date or at any other specified period different than the reference period for CPI. The CPI is therefore defined by

$$\mathrm{CPI}_{\mathrm{N}} = \frac{NW_{\mathrm{N}}}{RW} \tag{7.44}$$

where the subscript N indicates that the CPI and the NW correspond to the year N after (or before) the reference period.

Table 7.12 Equations for economic analysis

Parameter	Equation	Description
Market discount rate	$r_{\mathrm{m}} = (r+1)(i+1)-1$	The discount rate taking into account the inflation rate
Present value factor	$PVF = (1+r_{\mathrm{m}})^{-N}$	A factor used to determine the present value of cash flow
Capital recovery factor	$CRF = \frac{r_{\mathrm{m}}}{1-PVF}$	The ratio of a constant annuity to the present value of receiving that annuity for a given number of discount periods
Present worth factor	$PWF = CRF^{-1}$	A factor used to determine the present value of a series of values
Present worth income (\$)	$PWI = LPP\ AP\ PWF$	The income from a business expressed in the present worth of money. This is equal to cost output from product selling
Present worth costs (\$)	$\mathcal{C}_{\mathrm{in}} = LCC\ AC\ PWF$	This is a cost input due to the cost of fuels and supplies
Cost of O & M (operation and maintenance)	$\mathcal{C}_{\mathrm{o}\&m} = PWI\ OMCF$	Here, the O & M cost is taken as a fraction of income from product sales
Net income (\$)	$NI = PWI - \mathcal{C}_{\mathrm{o}\&m} - \mathcal{C}_{\mathrm{in}}$	Income from a business expressed in present worth
Tax credit deduction (\$)	$TCD = t_{\mathrm{c}}\mathcal{C}_{\mathrm{cap}}$	Tax deduction due to investment in renewable energy
Taxable income (\$)	$TI = NI - TCD$	The amount of income subjected to taxation
Tax on income (\$)	$TOI = t_{\mathrm{I}}TI$	The tax applied to the income
Tax on property(\$)	$TOP = t_{\mathrm{p}}\mathcal{C}_{\mathrm{cap}}(1-t_{\mathrm{i}})$	Tax applied on the property
Other cost creation	$\mathcal{C}_{\mathrm{occ}} = TOI + TOP$	The cost creation to support taxation on income and property
Generated costs (\$)	$\mathcal{C}_{\mathrm{gen}} = \mathcal{C}_{\mathrm{cap}} + \mathcal{C}_{\mathrm{o}\&m} + \mathcal{C}_{\mathrm{occ}}$	This is the total costs generated by the system during lifetime
Salvage value (\$)	$SV = CSF\ \mathcal{C}_{\mathrm{cap}}PVF(1-t_{\mathrm{s}})$	Salvage value expressed in present worth
Generated capital (\$)	$GC = NI + SV - \mathcal{C}_{\mathrm{cap}} - TOI - TOP$	Generated capital is equal to the accumulated cost within the system, according to the cost balance
Capital productivity	$CP = (\mathcal{C}_{\mathrm{cap}} + GC)/\mathcal{C}_{\mathrm{cap}}$	This factor compares the amount of available cash at the end of the lifetime $\mathcal{C}_{\mathrm{cap}} + GC$ to the invested equity capital

It is important to account for inflation when adopting a discount rate in any engineering project that extends over a predictable period in the future. Assume that for a given period of time, the inflation rate is i and the discount rate is r. Then, due to the productivity of capital, the future worth increases by $(1+r)$ times, while due to inflation, it decreases by $(1+i)$ times. Table 7.12 gives the equation for real rate in the form of the real discount rate. In engineering economics, it is recommended to pursue the analysis in *constant currency* (or real currency) that represents currency amended for the inflation. Therefore, in the calculation of present worth and compound amount factors and other economic indicators, the real discount rate must be used and not the market discount rate.

Inflation rate is calculated based on the average price of a basket of goods and services. However, some commodities including fuel and electricity display a real growth; that is, their price escalades more than the average price, represented by inflation. As a consequence, for a more accurate economic analysis, the price escalation of fossil fuels and electrical energy must be accounted for.

It is customary in economics to express costs and revenues that occur once or in irregular intervals as equivalent equal payments in regular intervals. This is beneficial in many situations: comparing the levelized cost of economic activities that extend over different period, establishing the rate on energy or electricity, computing loan rates, etc. This practice is known as *levelizing*.

The picture of economic analysis of any energy project is influenced by laws regarding taxation. In any society (or economic context), taxation is practiced for purposes such as (i) infrastructure works, education, health services, army, justice, and other basic social services administered by governments; (ii) redistribution of revenue toward undeveloped regions or industrial/social sectors; and (iii) repricing certain activities—for example, carbon emissions.

The purpose of this section is to present the general means to compute taxes as a part of the life cycle cost of any energy system.

- *Income tax*. In order to introduce the general taxation method, assume that at the end of the fiscal year an entity reports the total obtained taxable income I_t during that year. The income tax required by the law is a fraction t of the taxable income. Therefore, the considered entity has to pay the amount $T=I_t\times t$, where t is the tax rate. In order to determine the taxable income, a deduction D can be subtracted from the total income I; therefore, $I_t=I-D$. Relevant to life cycle analysis is the fact that some of the expenses (e.g., loans interest) are tax deductible. Assume that the amount C_t is tax deductible from the inventory of a project's life cycle cost. Then, the amount $D_t=t\times C_t$ represents the tax deduction and can be extracted from the life cycle cost.
- *Tax credit*. If the economic entity deploys a certain category of business (e.g., generates energy from renewable sources) it might be eligible for a tax credit. In this case, the income tax that the entity has to pay is reduced with an amount proportional to the investment in the tax credit activity. If C denotes the investment in a tax creditable activity, then the deduction received due to tax credit is $D_{cred}=t_{cred}\times C$, where t_{cred} is the tax on credit. In some countries, the tax credit on

renewable energy can go up to 40 % (see rabl, 1985). The amount D_{cred} should be extracted from the initial cost of the project.

- *Property tax*. Assume that a property is possessed by an economic entity, be it a business, a society, or an individual. In this case, a tax on the property (denoted here with t_{prop}) has to be paid to the regulated authority. This tax is deductible as income tax.
- *Carbon tax*. It is certain that most of governments will impose (some already do) tax on CO_2 emission such that the investment and consumption decision of the economic agents could be modified for the benefit of a better environment.
- *Depreciation*. It is a tax deduction due to the fact that, according to law, the worth of some categories of goods depreciates in time. Say that a good has a capital value C_{i} at time zero; after a period of time, its worth will depreciate with the amount C_{Dep}; then, the current worth becomes C_{i}–C_{Dep}. Since from the point of view of depreciation, the capital is a property and its worth diminishes over time, it comes out that each year a tax deduction can be obtained from depreciation.
- *Tax on salvage*. At the end of the lifetime, the system has a depreciated value known as the *salvage value* in economics. The tax perceived by the government when salvage is valorized, t_{salv}, is in general different than the income tax. Therefore, the factor $(1-t_{\mathrm{salv}})$ represents the amount of money that the business earns after tax, amount which discounts the capital investment.

Loans are paid in regular installments over a period of time N_{Loan} and with a real interest rate r_{Loan}, defined by loan agreement. The cost of loan is discounted by the business rate real discount rate r_{r}; therefore, using capital recovery factor, the cost of loan whose present value is C is given as follows:

$$C_{\mathrm{Loan}} = \frac{CRF_{(r_{\mathrm{Loan}},\, N_{\mathrm{Loan}})}}{CRF_{(r_{\mathrm{r}},\, N_{\mathrm{Loan}})}} C \tag{7.45}$$

where CRF is the capital recovery factor given in Table 7.12, N_{Loan} is the period over which the loan is given, r_{Loan} is the interest rate for the loan, and r_{r} is the real discount rate.

The basis of financing and economics presented in the above section allow for defining a number of useful criteria that can be used for technical and economical evaluation of a sustainable energy system. Furthermore, through these criteria, it is possible to perform system design optimization or one may use them for system selection among various options. In order, one briefly introduces the following criteria: life cycle cost, life cycle savings, internal rate of return, and payback period as follows:

- *Life cycle cost*. This represent the total cost of the system and is mainly divided into two parts: initial cost and periodic cost. The initial costs are mainly owing (or capital costs), while the periodic costs include operating and maintenance costs.

- *Life cycle savings*. The *life cycle savings* are defined as the difference between the cost savings on conventional fuel and the capital cost of the renewable energy system that is supposed to replace (or compete with) the energy system based on fossil fuel.
- *Internal rate of return*. It represents the rate of return for which the life cycle savings are nil. Internal rate of return is useful for comparing investments when the discount rate cannot be evaluated. If the real internal rate of return is higher than the average real rate of return on similar investments, then the considered business is profitable.
- *Payback period*. The period defined as the ratio of capital cost over annual savings. In other words, the investment in the system is paid by the savings at the end of the payback period.

Based on the assumption of equivalent total fuel energy input for the mixed fueling cases, the reduction in CO_2 is determined for each fuel blend. The GF is a useful parameter for the comparison of the fuel blends with the base diesel case, and with respect to locomotive emissions reduction, may be considered in decision-making and justification for the use of ammonia fueling.

For system comparison from a cost perspective in a railway clean air project, the estimated additional equipment costs and change in fuel cost can be compared to the diesel baseline case. Therefore, some cost factors can be derived for comparison purposes of newer technologies. For example, a fuel cost factor can be introduced as defined by the current price of the alternative fuel divided by the price of the baseline ULSD fuel. Thence, this factor is calculated as follows:

$$CF_{\text{fuel}} = \left| 1 - \frac{C_{\text{fuel}}}{C_{\text{ULSD}}} \right. . \tag{7.46}$$

Regarding the equipment cost, the capital required for each of the novel systems proposed for a clean air project must be added to the baseline price of the locomotive. Therefore, an equipment cost factor can be introduced as follows:

$$CF_{\text{eq}} = \left| 1 - \frac{C_{\text{new}} + C_{\text{ref}}}{C_{\text{ref}}} \right. \tag{7.47}$$

where C_{ref} is the present value of the locomotive considered, and C_{new} is the sum of the costs for the additional components.

7.7 Closing Remarks

In this chapter, the analysis and assessment methods applicable to locomotive systems are presented and discussed. Thermodynamic analysis stands at the base of any analysis and assessment activity for any system. This analysis can only be achieved by energy and exergy methods through EBE and ExBE. Energy analysis is beneficial for comparative assessment of systems and processes with respect to the ideal case of reversible operation under the conservation law. However, in exergy analysis, the interaction of the system with the environment is intrinsically considered. This is a great feature of the exergy method allowing for its expansion and combination with the environmental impact assessment and economic analyses.

Furthermore, the most relevant thermodynamic power cycles such as Otto, Diesel, dual cycle, and Brayton cycle are presented in view of the analysis of locomotive systems. An important aspect is the definition of power generation efficiency through energy and exergy. Other locomotive-specific assessment indicators are presented within the chapter. The environmental and economic analyses are reviewed in sufficient extend to facilitate the understanding of Chap. 8 of this book where several assessment case studies are presented for potential clean rail options.

Chapter 8
Case Studies

8.1 Introduction

The extensive use of fossil fuel in the railway transportation is of a great concern worldwide, particularly in North America where diesel and/or diesel-electric locomotives represent the majority of the prime movers. Besides rail transport, a major emission source of greenhouse gases is road transportation, which relates practically to gasoline and diesel fuels. As an example, in Canada, the transportation sector is the largest contributor to the greenhouse gas emissions (GHGs) with over 25 % of the total emissions. Reduction of these emissions—among other important factors—s a strong encouragement for public transit, especially rail transit, for the benefit of cleaner air and better environment. This obviously implies development and implementation of a clean rail transportation infrastructure.

This book discusses the current status and historical overview of rail transport and rail transport systems and applications, and the development of alternative system and fuel options for a clean rail sector that relates to the sustainable energy sources and fuels, and thus produces substantially less pollution than the conventional railway, which is in place today. Various cleaner fuels are considered in the past among which one notes natural gas (in compressed or liquefied forms), methanol and biodiesel or other diesel fuel blends, hydrogen, and more recently ammonia. Purely electric rail transport remains a major option, which although being expensive, it may be the preferred solution for some jurisdictions related to clean power generation (e.g., hydro, wind, and nuclear).

This chapter details the thermodynamic, environmental, and economic assessments and results for each of the locomotive systems described in Chap. 6. The conventional diesel-fueled locomotive is the performance baseline against which alternative systems are compared, with respect to fuel and emissions, energy utilization, and system cost. Each alternative addresses the opportunities for energy recovery from heat otherwise lost in exhaust gases and cooling water, considering both the first and second laws of thermodynamics. This gives a comprehensive and objec-

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tive method for quantification of the available energy for recovery, and the overall benefit of the system improvements by considering energy and exergy efficiencies against the environmental impact reduction and cost of the additional components.

Ammonia is applicable as a carbon-free combustion fuel, heat transfer and/or recovery fluid, and working fluid for the locomotive and integrated subsystems for the alternative locomotive options under consideration. This is a significant advantage; one storage tank serves multiple applications, minimizing additional weight otherwise required for multiple fluids and storage tanks to supply the additional subprocesses and/or subsystems. Of the alternative systems, there are three general categories: alternative fueling, energy recovery via integrated power generation subprocesses, and energy recovery applications via integrated subsystems. These categories are addressed as case studies for the various ammonia-based alternative systems, subsequent to the assessment of the baseline diesel locomotive.

8.2 General Assumptions and the Prime Mover Internal Combustion Engines (ICE) Modeling

The prime mover sizing and the operating conditions for the locomotive engine introduced in Table 6.2 are reiterated in Table 8.1 along with additional details; including maximum cylinder pressure, engine cooling heat removal rates, and temperature levels of cooling water circuits. These details, based on known and derived information for the same and similar locomotives (for further information, refer to [34, 106]) give a basis for the systems modeling and analysis. The following general assumptions are made in the systems modeling and analysis:

- Locomotive operates at rated conditions.
- All subprocesses and subsystems operate at steady state.

Table 8.1 The prime mover sizing details and the locomotive operating conditions (Sources: [32, 90, 91])

Engine model (EMD)		16V-710G3
Traction power, THP (hp) [W_{TP}] (kW)		4000 [2983]
Engine speed, N_{ICE} (rpm)		900
Brake mean effective pressure, bmep (kPa)		1069
Displacement volume per cylinder, V_d (L)		11.635
Compression ratio, r		16:1
Bore (m)		0.23019
Stroke (m)		0.2794
Number of cylinders, n_{cyl}		16
Fuel tank volume, V (L)		8410
Turbocharger pressure boost, p_{TC}		1.25
Maximum cooling water reservoir temperature, T_{CW} (°C)		49
Maximum engine jacket cooling water Outlet Temperature T_{12} (°C)		85
Heat removal rate[a]	Water jacket cooling, HRR_{wjc} (kJ/kW$_{TP}$·h)	2377
	Aftercooler, HRR_{ac} (kJ/kW$_{TP}$ h)	908
Maximum cylinder pressure, P_{max} (kPa)		10,800

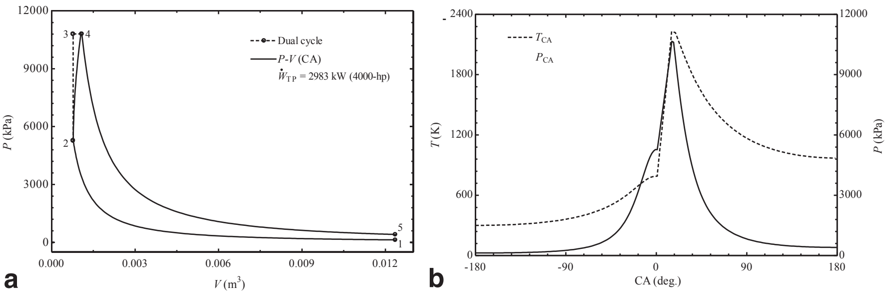

Fig. 8.1 The prime mover ICE **a** two-stroke dual cycle, and **b** cylinder temperature and pressure for one crankshaft revolution

- Auxiliary component pressure losses are negligible.
- Additional turbines and compressors have isentropic efficiencies (η_s) of 0.75.

The thermodynamic cycle and the instantaneous pressure and temperature for the two-stroke compression ignition ICE are shown in Fig. 8.1 at rated operating conditions and with diesel fueling. Brake-specific fuel consumption is calculated to be 0.255 kg/kW h for the lean case ($\varphi = 0.9$), which is consistent with other studies for the same locomotive prime mover [20, 107, 108] . The prime mover ICE model is applied for each of the locomotive systems to assess the performance, and quantify the energy and exergy values of waste heat streams for integration of the subprocesses and subsystems for the alternative systems.

8.3 Conventional Diesel-Electric Locomotive

Locomotive system 1 is shown in Fig. 8.1, representing the diesel-fueled case operating at rated conditions. From the prime mover ICE modeling results, the locomotive prime mover has an energy efficiency, $\eta_1 = 0.33$, and an exergy efficiency, $\psi_1 = 0.308$. Heat is partially recovered from the exhaust gases leaving the ICE by the turbocharger unit; intake air is compressed and then cooled (in the aftercooler) prior to entering the engine intake manifold to increase the total mass flow rate of air into the engine. The two-stroke diesel locomotive engine produces shaft power to directly drive the auxiliary system components; including air compressors, fuel and coolant pumps, and the main and auxiliary generators. The generator(s) convert mechanical work to electricity with an assumed conversion efficiency of 0.95 [109]. The main generator supplies power to the electric motors, producing traction power at a rate of 2983 kW (4000 hp) at an engine speed of 900 rpm (Fig. 8.2).

Energetic and Exergetic Assessment The energy balance for system 1 is shown in Fig. 8.3. The rate of exhaust heat energy ($\dot{Q}_{exh}$) represents that of the gases following turbocharger process at state point 5. Heat removal from the engine body and turbocharger aftercooling is primarily done by transferring to the cooling water circuits, which is subsequently cooled by radiator fans. These losses account for nearly two thirds of the total energy input by diesel fuel. Internal energy consumption is

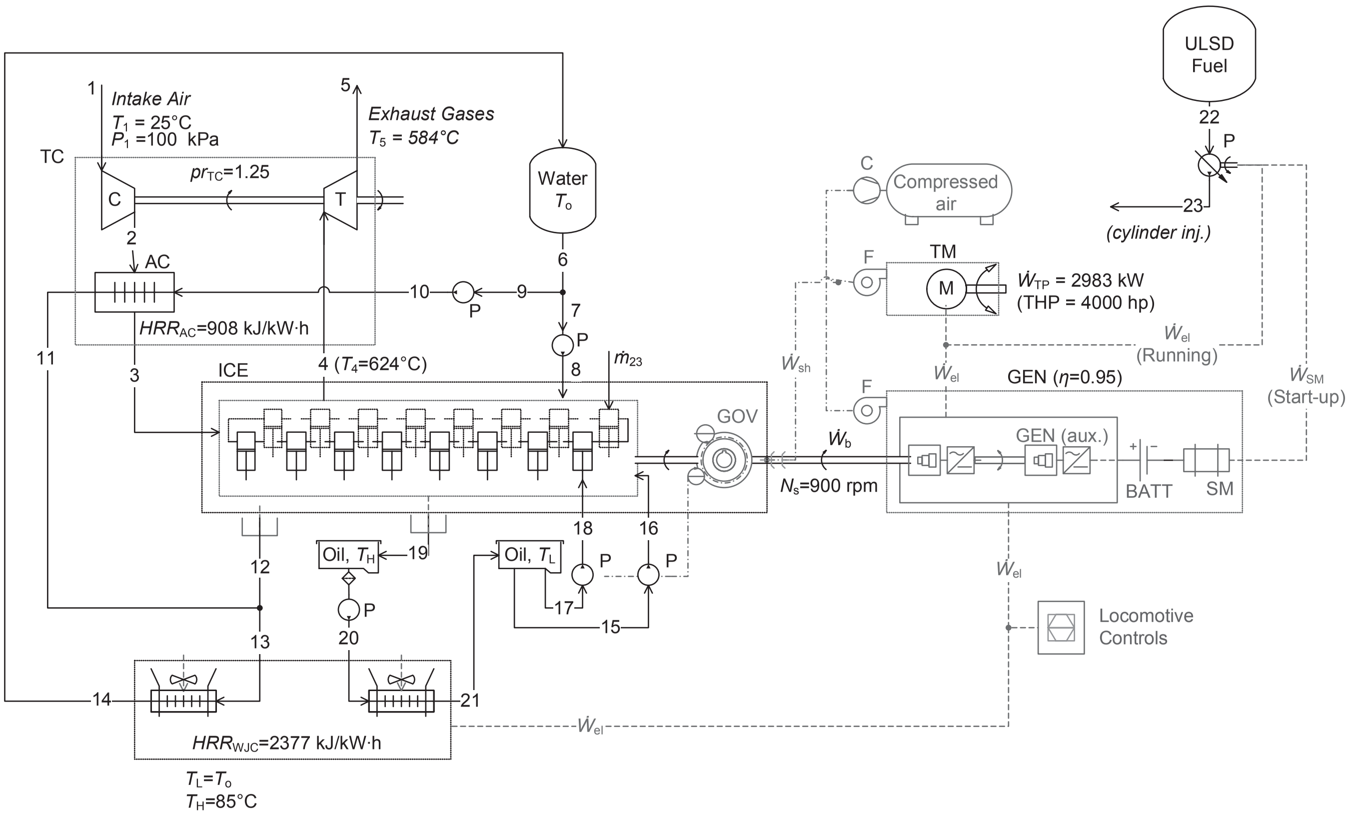

Fig. 8.2 Diesel-fueled locomotive (system 1)

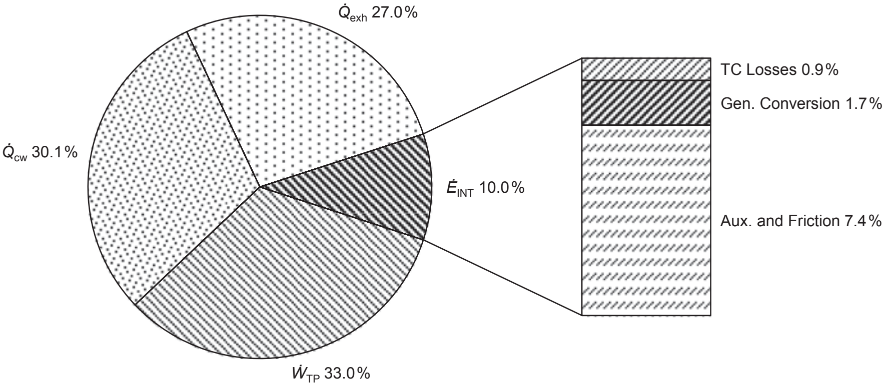

Fig. 8.3 Energy balance of locomotive system 1 ($\eta_1 = 0.33$)

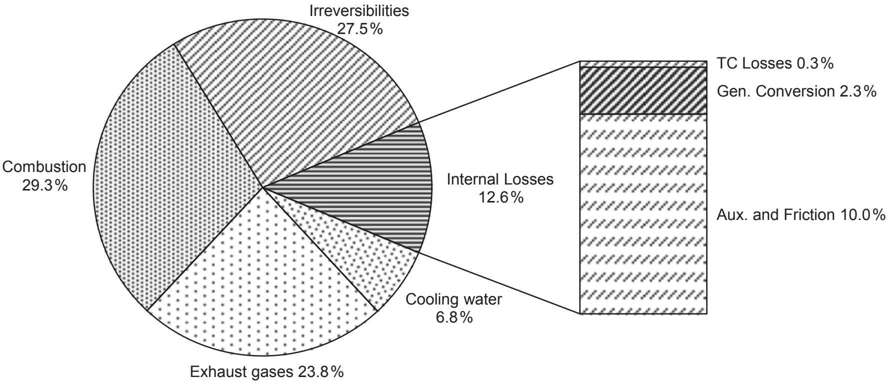

Fig. 8.4 System 1 exergy destruction ratios of internal and external losses ($\psi_1 = 0.308$)

taken as the total for the work losses of the turbocharger, generator conversion, friction, and auxiliary processes.

To identify and quantify heat recovery options for potential NH_3 subsystems, it is necessary to evaluate the quality of the waste heat sources through exergy analysis. Although the amount of energy of a given source may indicate potential for recovery, its temperature is a limiting factor, particularly for mid to low temperature heat sources such as the cooling water. The exergy values of the system losses and irreversibilities are given as a ratio of total exergy destruction in Fig. 8.4 to identify energy recovery opportunities.

8.4 Ammonia-Based Alternative Locomotive Case Studies

Case Study I: Ammonia-Diesel Co-Fueling Options The additional NH_3 processes for systems 2 and 3 are shown in Figs. 8.5 and 8.6. Exhaust treatment by the selective catalytic reduction (SCR) requires pressure reduction by throttling of the

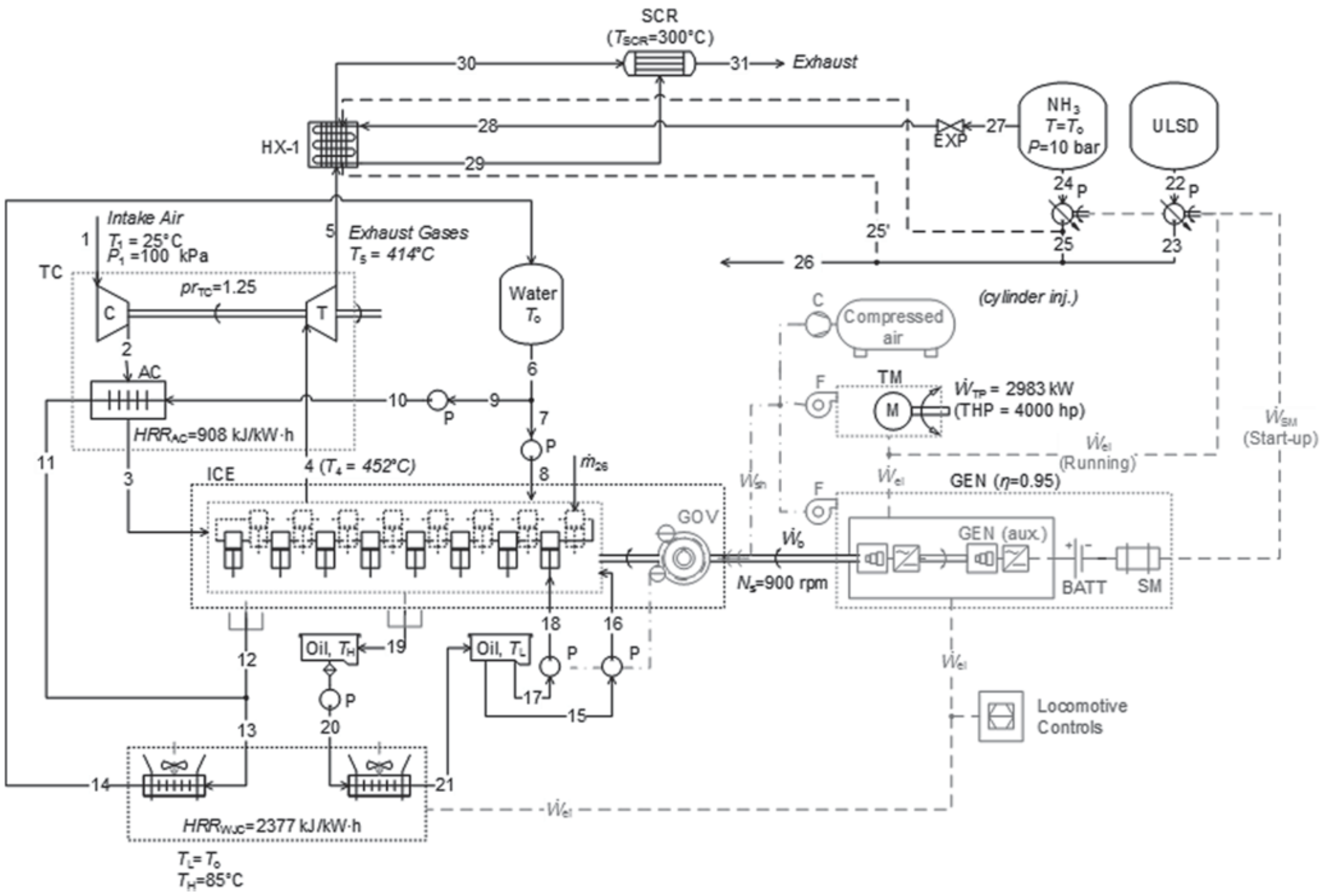

Fig. 8.5 NH_3 co-fueling and exhaust gas selective catalytic reduction (SCR) (system 2)

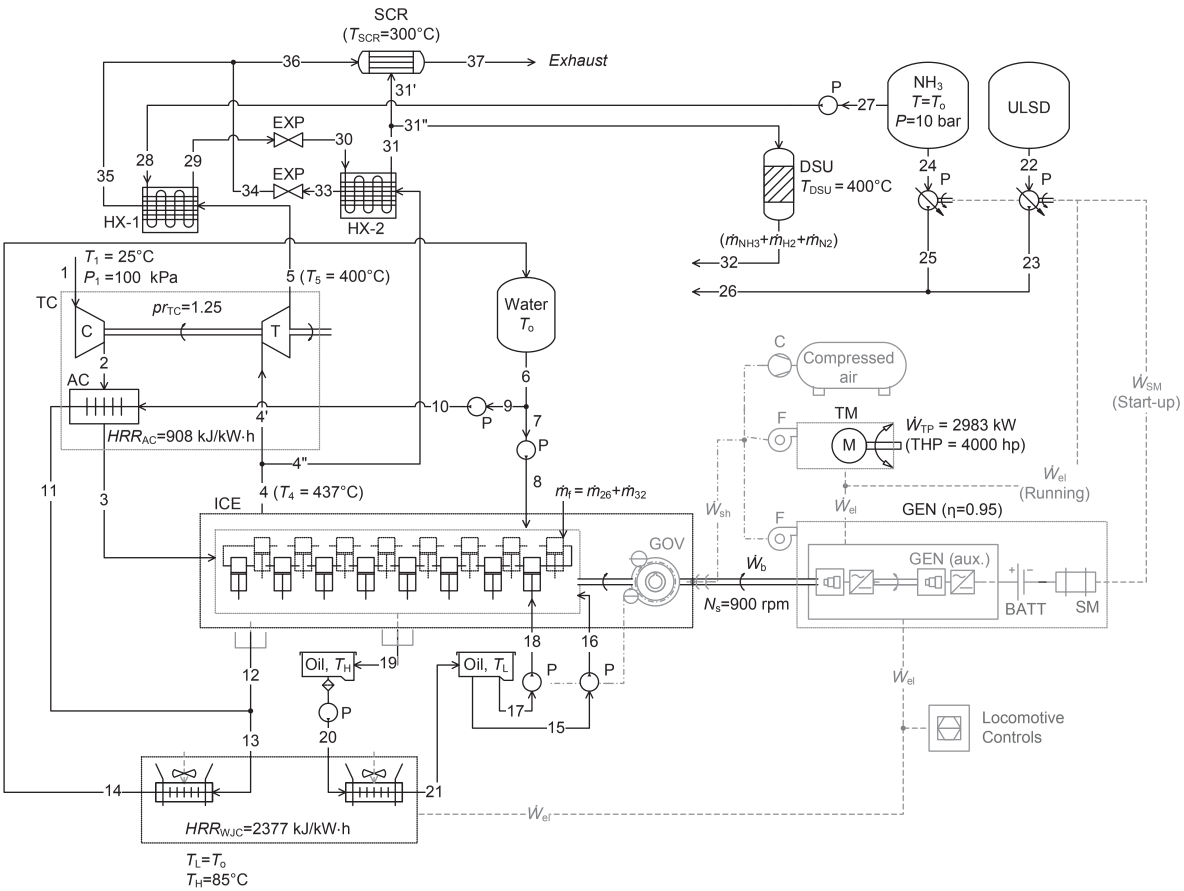

Fig. 8.6 NH_3 co-fueling and decomposition for onboard H_2-fuel production (system 3)

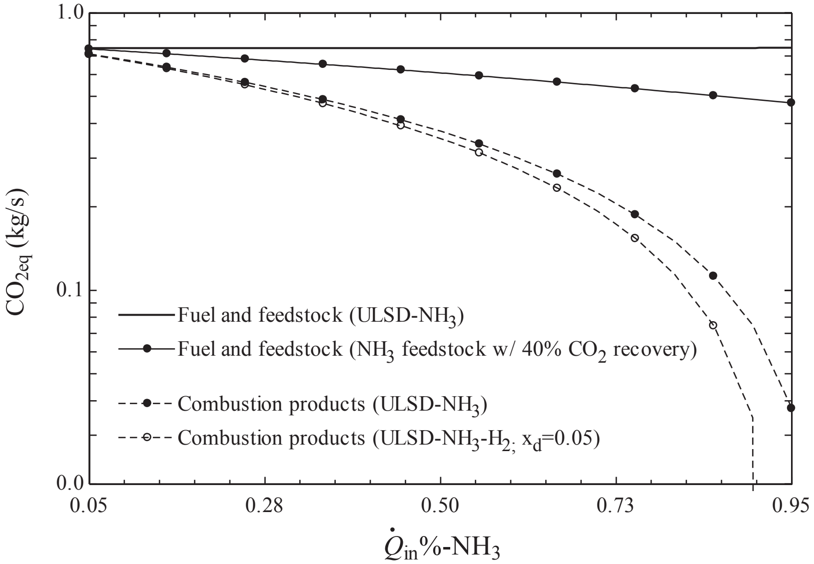

Fig. 8.7 Greenhouse gas emissions (GHG) emissions including fuel production (lifecycle), and combustion-only for varying NH_3-ULSD fuel blends

ammonia supply to the operating pressure of the SCR unit, occurring across state points 27–28 in system 2, and 33–34 in system 3. Exhaust heat recovery raises the temperature of NH_3 prior to injection into the SCR, and preheating of NH_3 fuel prior to combustion.

GHG and CAC Emissions for NH_3 Co-Fueling Emission reduction by co-fueling with NH_3 are plotted against the fraction of NH_3 fueling in the subsequent figures. GHG emissions are shown in Fig. 8.7, considering only the production-related emissions for NH_3 production by natural gas with and without CO_2 capture in and for combustion products only. The results clearly indicate the importance of production-related CO_2 on the environmental impact of NH_3, and support the use of renewable energy systems for the production of NH_3 fuel to provide carbon-free (or carbon-minimum) fuel.

Reduction of criteria air contaminants (CAC) emissions with and without SCR are shown in the Figs. 8.8 to 8.11 with respect to the set tier 2, 3, and 4 emission limits—previously listed in Table 2.2—to give an indication of the benefit of investing in the alternative fuel and SCR technologies, since the current optional locomotive retrofits and upgrades to reduce emissions will eventually become necessary as increasingly strict limits are imposed.

The level of NO_x emissions (Fig. 8.8) is well below tier 2 and tier 3 limits, and even without SCR the emission reductions are achieved with approximately 50 % of fuel input supplied by NH_3. Similar results are found for the PM emissions (Fig. 8.9). The range of CO emissions (Fig. 8.10) indicates the reduction below tier 2, 3, and 4 limits for all the fuel cases considered, with the maximum reduction achieved by NH_3-ULSD fueling including SCR. Hydrocarbon (HC) emission

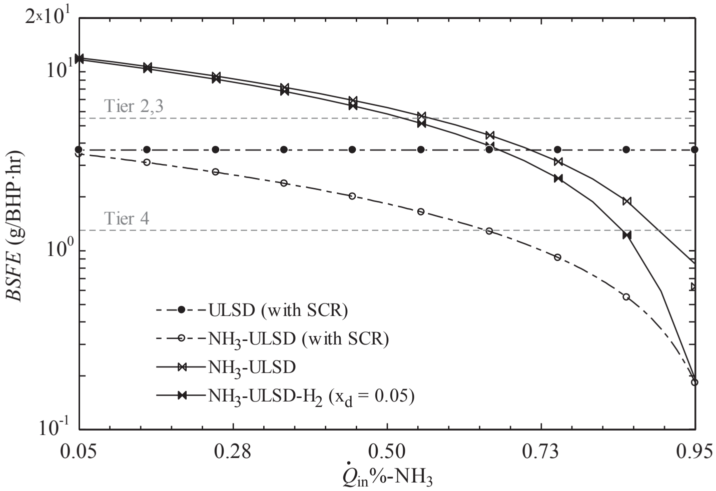

Fig. 8.8 Brake-specific NO_x emissions for varying NH_3 fuel-energy fraction

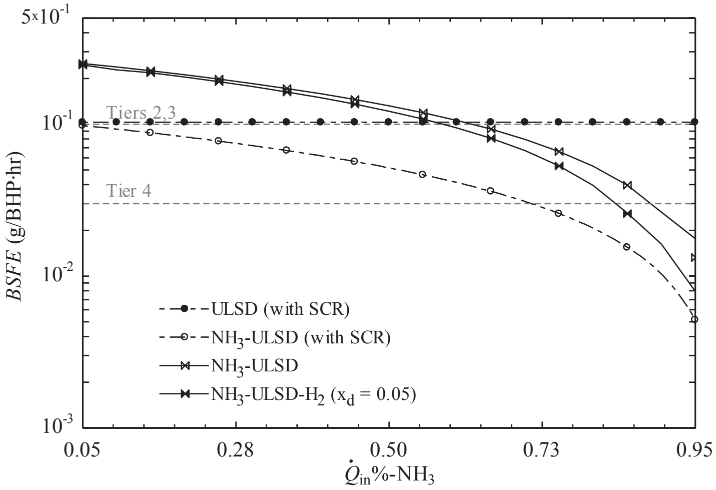

Fig. 8.9 Brake-specific PM emissions for varying NH_3 fuel-energy fraction

reductions are shown in Fig. 8.11, showing emissions below tier 2 and tier 3 limits achieved with approximately 50 % of fuel energy input supplied by NH_3 without the SCR unit, and approach tier 4 limits for the mixed fuel case with SCR integration for the same NH_3 fuel-energy fraction.

Energy and Exergy Assessments The variation of exhaust temperatures at the ICE and turbocharger exits are plotted in Fig. 8.12 to indicate the range over which the temperature remains above the sufficient level to supply heat for the DSU process in order to produce H_2 fuel. There is a sharp decrease in temperature, as the NH_3 fuel-energy fraction approaches 50 %, after which the exhaust temperature falls

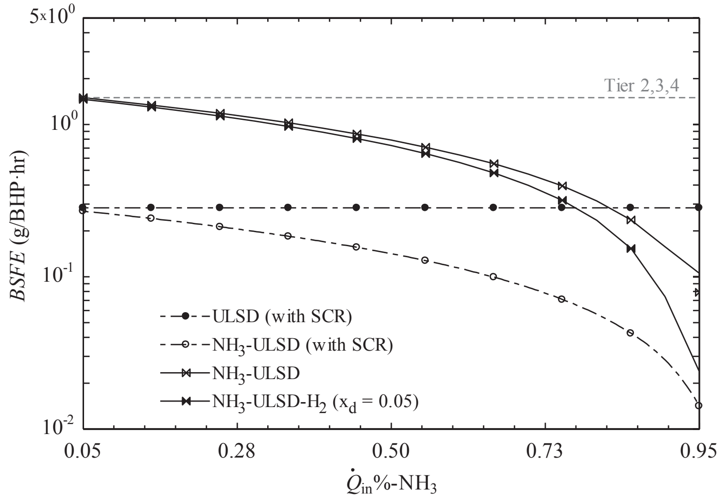

Fig. 8.10 Brake-specific CO emissions for varying NH_3 fuel-energy fraction

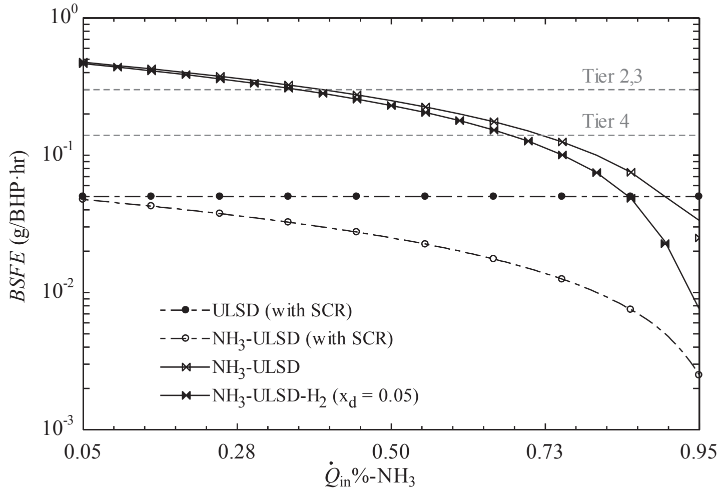

Fig. 8.11 Brake-specific hydrocarbon (HC) emissions for varying NH_3 fuel-energy fraction

below the levels of the DSU operating temperature (400 °C), limiting heat recovery for alternative configurations. Furthermore, without ignition assistance from either diesel or H_2 fuel to initiate combustion, the spark resistant and slow burning nature of NH_3 poses operating issues that can increase the resulting amount of unburned fuel in the exhaust, and thus reduce the shaft power production to drive the traction motors.

Based on the emission reductions and the exhaust temperature requirements to maintain operation of the DSU and SCR components at rated locomotive operation, a fraction of 50 % NH_3 fueling is assumed for the systems. The resulting fuel flow rates are listed in Table 8.2 for each fuel.

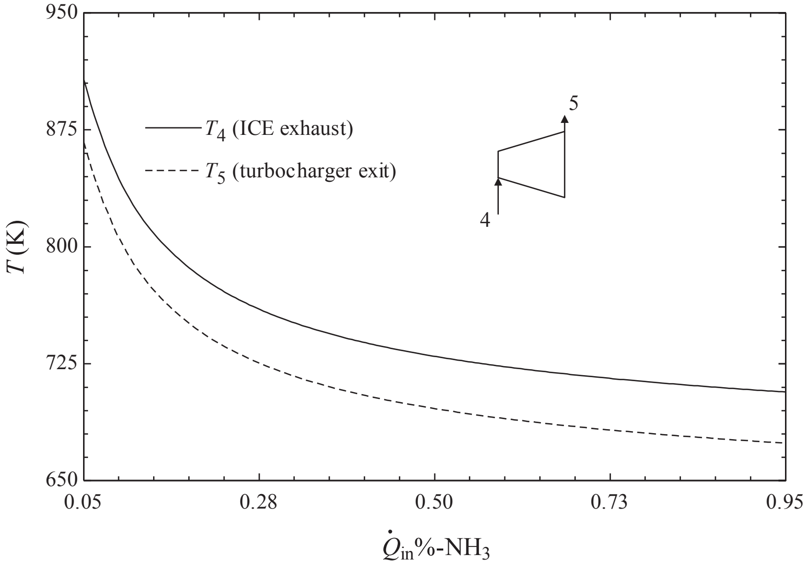

Fig. 8.12 Internal combustion engines (ICE) and the turbocharger exhaust temperatures for varying NH_3 fuel-energy fraction

Table 8.2 Fuel mass flow rates for diesel and NH_3 co-fueling cases

Fuel/blend	System	%-$\dot{Q}_{in}$ NH_3	x_d	$\dot{m}_{ULSD}$ (kg/s)	$\dot{m}_{NH3}$[a] (kg/s)	$\dot{m}_{H_2}$ (kg/s)
1	1	100% ULSD	–	0.212	–	–
2	2	50% NH_3	–	0.106	0.241	–
3	3–10	50% NH_3	0.05	0.0996	0.241	0.00225

[a] Flow rate of NH3 fuel only (does not include NH3 supplied to the SCR)

The heat recovery by NH_3 streams for the SCR and fuel supply are shown in Fig. 8.13 on a *T*-s diagram for ammonia. Liquid NH_3 is drawn from the tank at point 27 and throttled to atmospheric pressure at point 28. The liquid–vapor mixture is heated by exhaust gases in the exhaust recovery heat exchanger (HX-1) to the required temperature for the SCR at point 29.

If dual-fuel injection technology for liquid–gas fueling is integrated, the level of preheating (and, therefore, heat recovery) can be extended to saturated or superheated conditions for the NH_3 fuel stream, with associated heat recoveries ranging from approximately 250–425 kW-thermal. Four scenarios are considered in Table 8.3; SCR-NH_3 supply preheating (scenario A), SCR-NH_3+NH_3 fuel preheating to saturated liquid state (scenario B), SCR-NH_3+NH_3 fuel preheating to saturated vapor state (scenario C), and SCR-NH_3+NH_3 fuel preheating to superheated vapor state (scenario D).

The energy balance of the ICE is shown in Fig. 8.14 for scenario B, which does not necessarily require specialized equipment for gas–liquid fuel mixtures. The re-

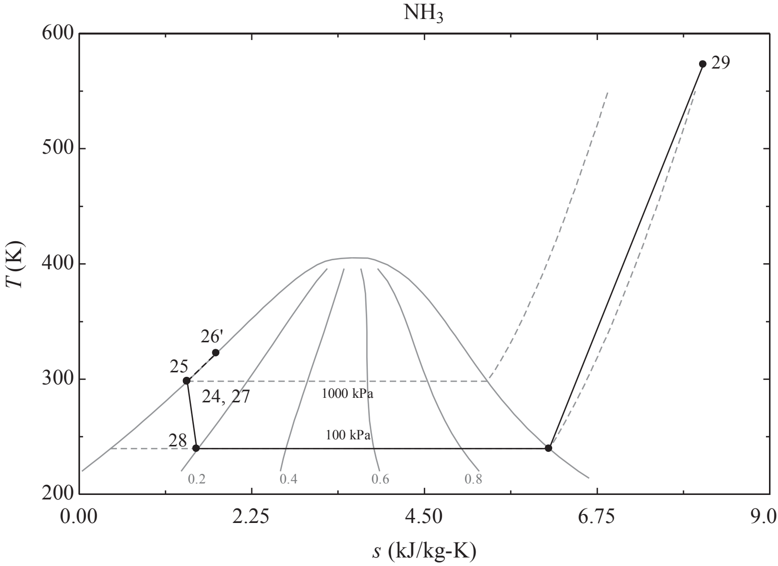

Fig. 8.13 *T-s* diagram of NH_3 processes for system 2

Table 8.3 Additional NH_3 process results for locomotive system 2

NH_3 fuel pump, $\dot{W}_{P2}$ (kW)		3.60
Heat recovery, $\dot{Q}_{Rec}$ (kW)	SCR supply preheat (scenario A)	7.48
	SCR supply + fuel preheat (scenario B: saturated NH_3 liquid)	122.6
	SCR supply + fuel preheat (scenario C: saturated NH_3 vapor)	262
	SCR supply + fuel preheat (scenario D: superheated)	437

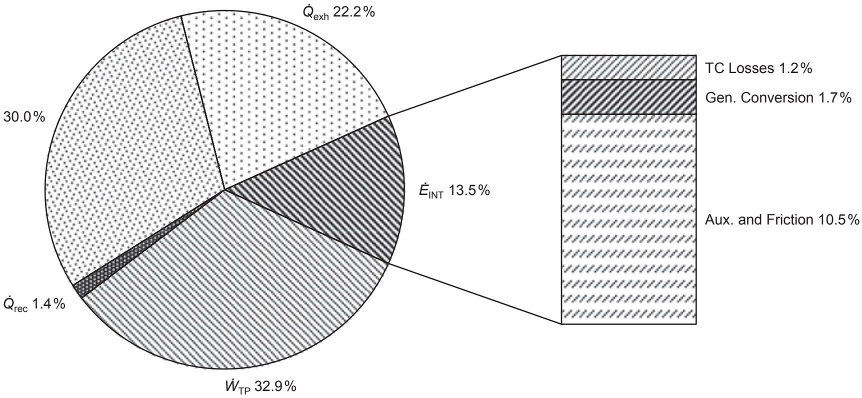

Fig. 8.14 System 2 energy balance ($\eta_2 = 0.343$)

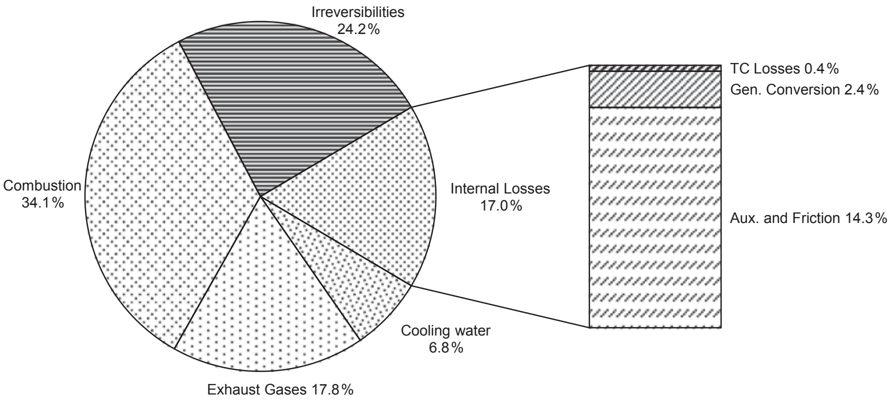

Fig. 8.15 Exergy destruction ratios for system 2 ($\psi_2 = 0.314$)

duction in exhaust energy available for recovery in HX1 relative to the baseline case is due to the lower exhaust temperature for the NH_3-ULSD fuel blend.

The exergy efficiency for system 2 is calculated to be 31.4%, and the exergy destructions are described in Fig. 8.15 using the exergy destruction ratios for the major points of loss. There is a higher rate of exergy destroyed in combustion than in the diesel-only case, due to the increased amount of energy required to burn NH_3, which has a lower flame speed and higher value for minimum ignition energy than diesel fuel. The internal (friction) losses are also higher, due to the higher volume flow of fuel than in the diesel-only case, thereby increasing the losses in the fluid flow and pumping.

If a wide range of NH_3 fueling is considered, fuel preheating in HX1 is limited by the minimum exhaust temperature for SCR-operating conditions (set to 300 °C). Superheating of the NH_3 gas is limited to temperature below the autoignition temperature of NH_3. The energy and exergy efficiencies for four scenarios are shown in Fig. 8.16 for a range of NH_3-ULSD fuel blends.

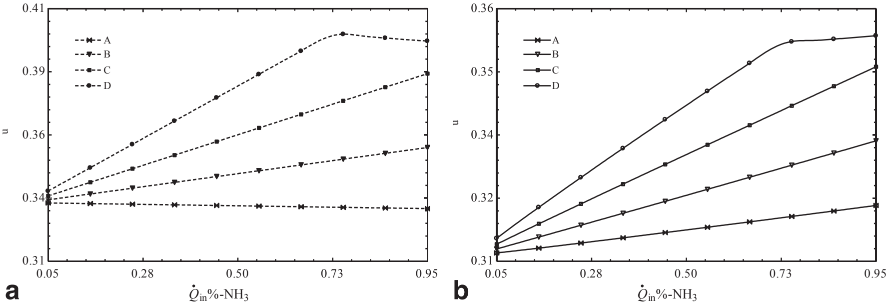

Fig. 8.16 **a** Energy, and **b** exergy utilization efficiencies for system 2, scenarios A–D

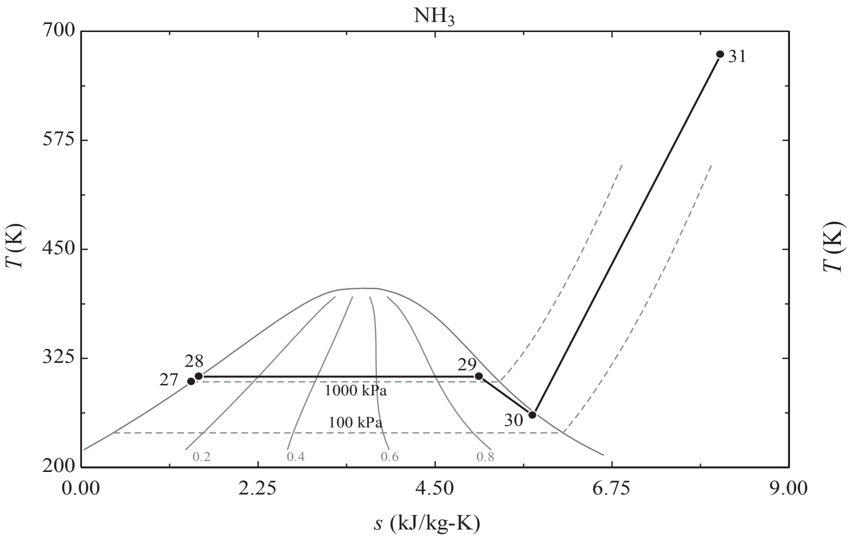

Fig. 8.17 *T-s* diagram of system 3 NH_3 process heat

System 3 introduces the thermal DSU, and an additional exhaust recovery heat exchanger (HX-2). The exhaust gas from the ICE is split into two streams, with a fraction directed to the turbine (T1) to maintain the required turbocharger operation, and the remaining fraction diverted to heat exchanger HX-2, to provide the final heating stage for the NH_3 stream. The total NH_3 fuel supply stream is sent through the heat exchangers to maximize the heat recovery. Figure 8.17 indicates the operations for system 3 integrated NH_3 heat recovery.

Heat recoveries from HX-1 raise the temperature of the NH_3 stream to the DSU operating temperature, with the useful heat given by the value of Δh_{DSU} calculated as described in Chap. 7. Another consideration is the compression, ($\dot{W}_{C2}$) of the product gases from the DSU required for cylinder injection into the ICE. It is assumed that the gases are cooled to approximately 80 °C prior to compression, to reduce the work requirement to compress the gases leaving the DSU.

The modeled energy efficiency is 33.8 % for system 3 and the energy balance is shown in Fig. 8.18. Energy recovery from exhaust supplies heat for the DSU process, though a portion of energy is spent on the compression of the DSU products for injection into the ICE intake, which is assumed to take place at 2000 kPa [110].

System 3 exergy efficiency is calculated as 30.9 %. As Fig. 8.19 indicates, the most significant exergy destructions occurring in combustion and heat transfer processes for the exhaust and coolant streams. The additional consumption by NH_3 subsystems and the compression of DSU products are also shown, making up the remaining portion of the exergy destructions.

System 4, shown in Fig. 8.20, operates in a similar manner as that of system 3, but introduces the option of additional work production by expansion of the N_2

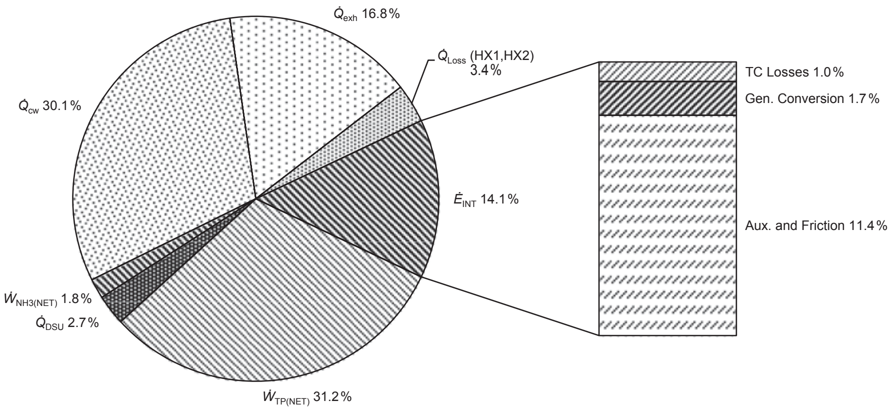

Fig. 8.18 System 3 energy balance ($\eta_3 = 0.339$)

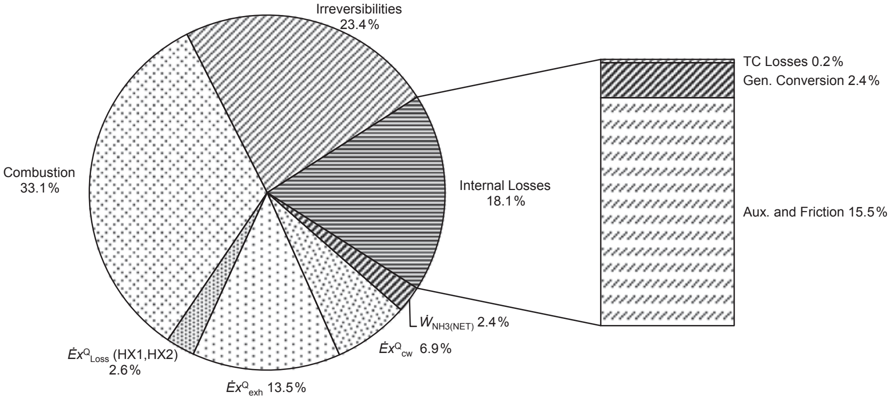

Fig. 8.19 Exergy destruction ratios for system 3 ($\psi_3 = 0.309$)

product stream. Following decomposition, N_2 gas is expanded in turbine T1 to produce additional work ($\dot{W}_{T2}$). The DSU in this system model operates at 200 kPa, with the final pressure after the N_2-expansion process at atmospheric pressure.

The system 4 energy balance is shown in Fig. 8.21, with energy efficiency determined to be 33.9 %, with a very slight gain from the system 3 efficiency due to the additional turbine work. The exergy efficiency for system 4 is calculated to be 31.0 %, which is a negligible increase from system 3. The losses are shown in Fig. 8.22, indicating that the additional expansion process loss and irreversibility system ultimately negates the benefit of the expansion work produced.

Case Study II: Ammonia-Based Energy Recovery Options The systems are shown in Figs. 8.23 and 8.24. The approach taken in system 5 uses a larger pressure ratio to increase the power produced by the turbine, recovering heat from exhaust gases from the turbocharger to superheat the ammonia stream. In the system 6 approach,

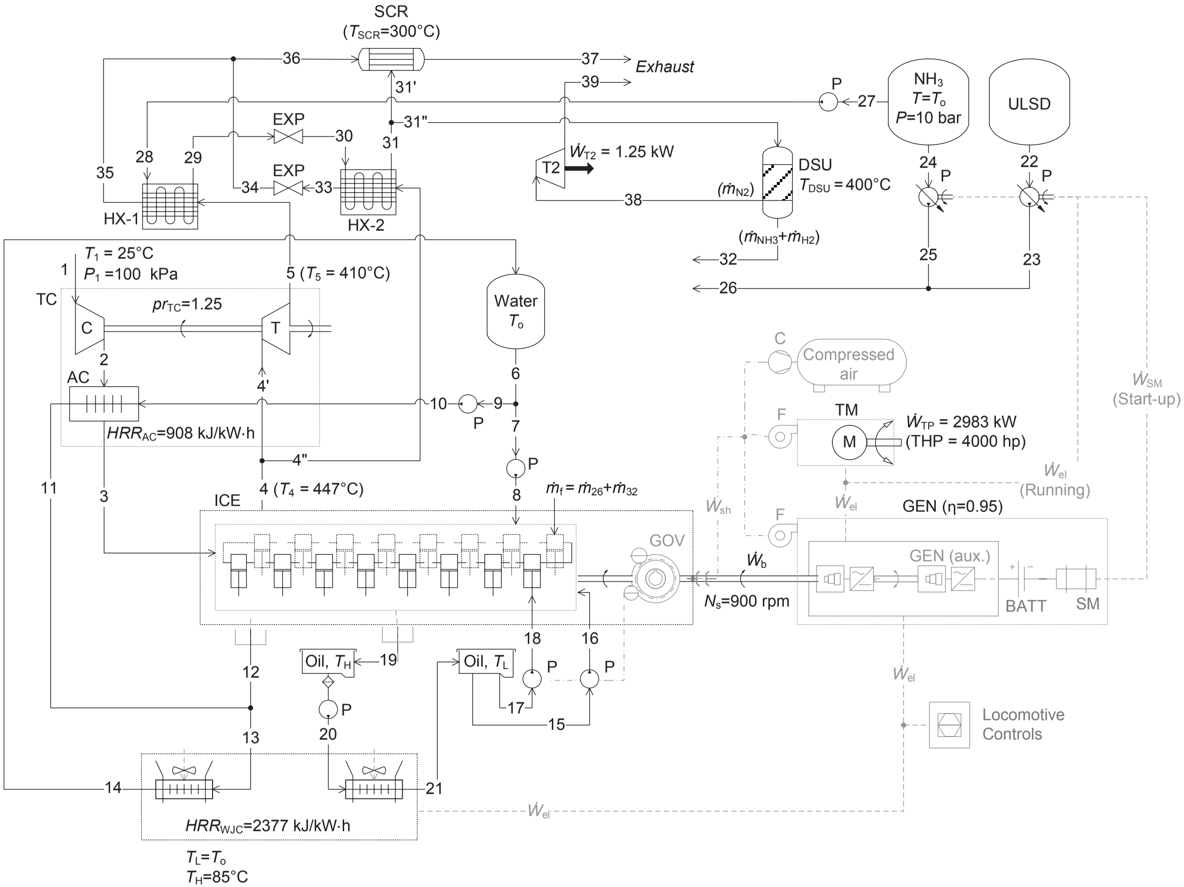

Fig. 8.20 NH$_3$ co-fueling and decomposition with N$_2$ expansion (system 4)

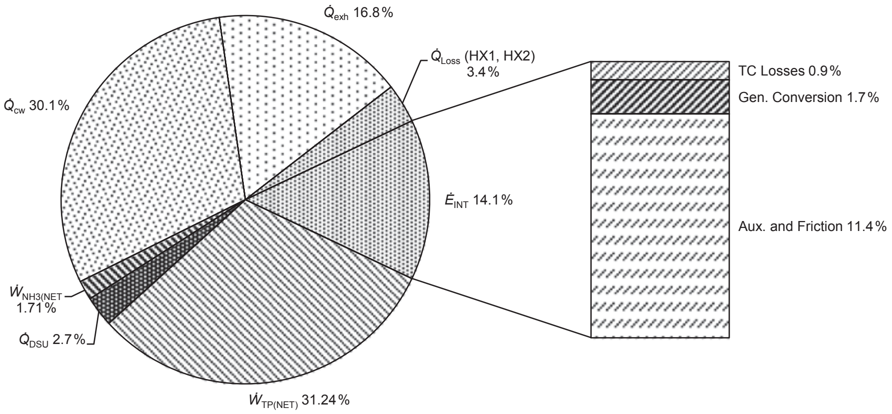

Fig. 8.21 System 4 energy balance ($\eta_4 = 0.339$)

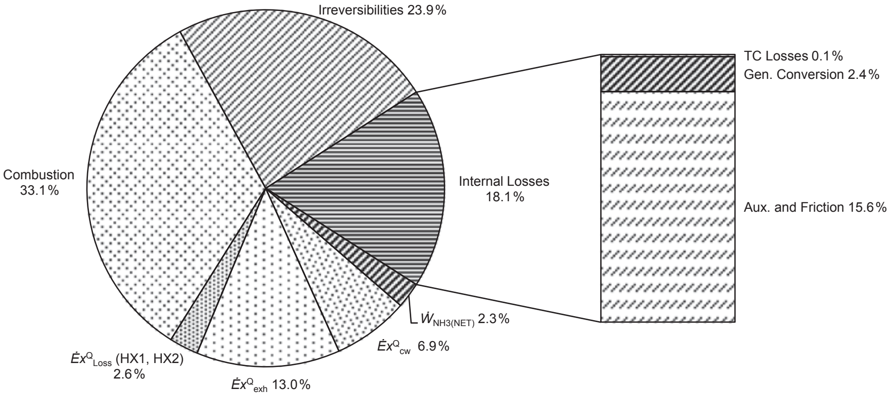

Fig. 8.22 Exergy destruction ratios for system 4 ($\psi_4 = 0.31$)

low-grade heat is recovered from the engine water jacket coolant (water) by reducing the pressure and temperature of the ammonia stream directed to the indirect engine cooling processin order to produce a saturated vapor, which can be superheated and expanded in multiple stages.

The ammonia processes for systems 5 and 6 are shown in Fig. 8.25a and b, respectively, and investigate the effect of multistage heat recovery, and multistage expansion processes on the performance of the system (Table 8.4).

The energy balance for system 5 is shown in Fig. 8.26, with a calculated energy efficiency of 34.5%. The increased power produced in the additional expansion processes reduces the impact of the compression requirements for the DSU product gases being sent to the engine intake.

The exergy efficiency for system 5 is calculated to be 31.6%, accounting for the losses that occur in the major ICE processes, as well as the additional NH_3 subsystems. The NH_3 system losses are most significant in the compression of DSU products, as well as in the large heat exchangers, as shown in Fig. 8.27.

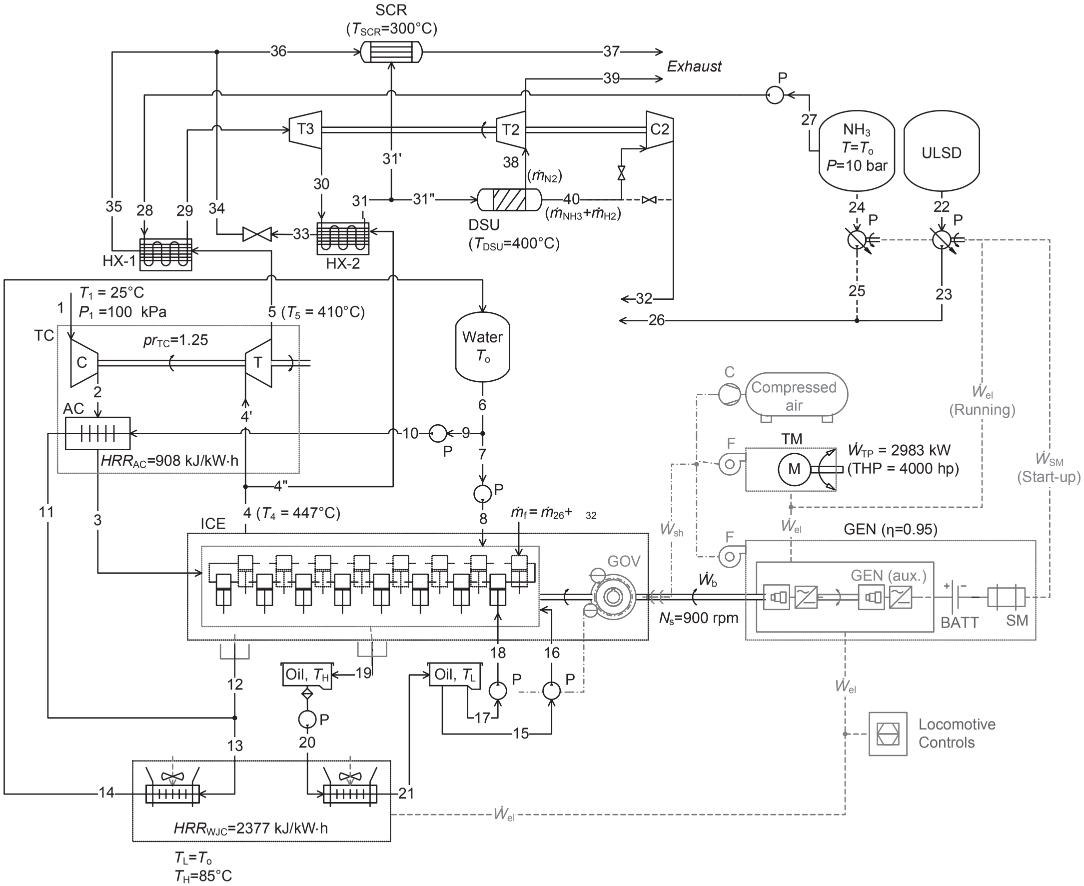

Fig. 8.23 NH_3 co-fueling and expansion work (system 5)

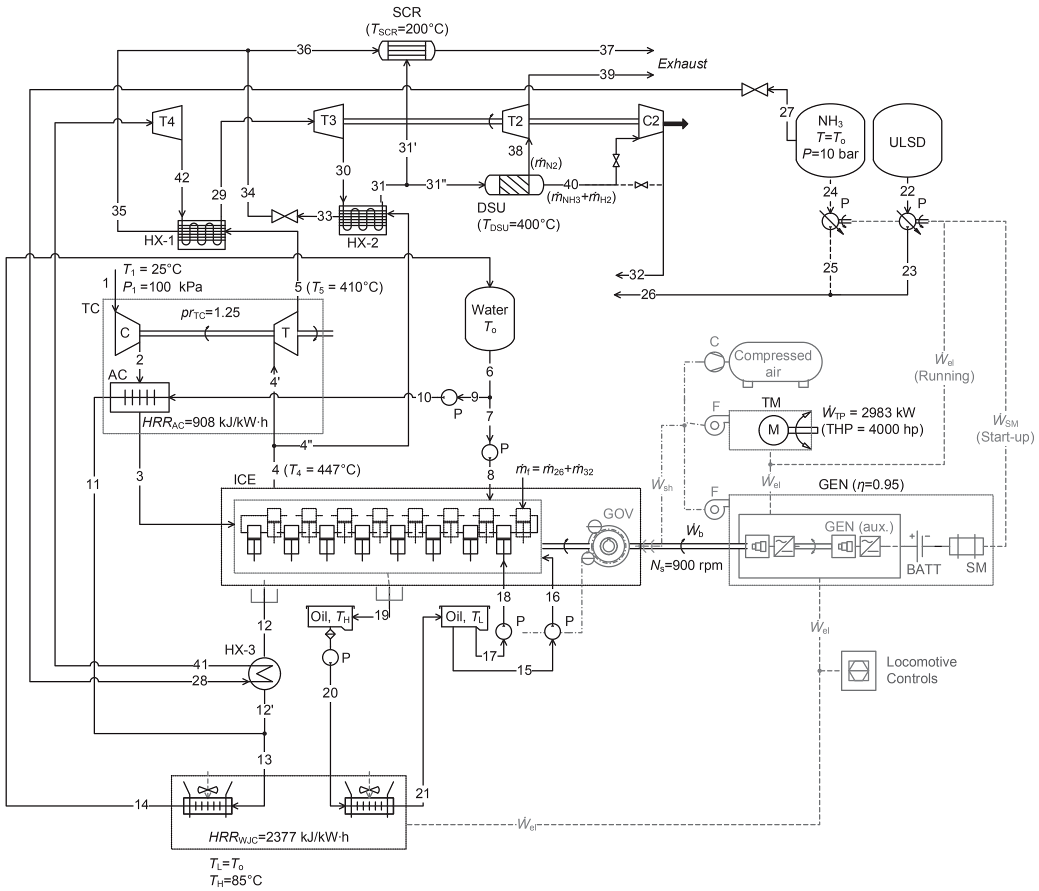

Fig. 8.24 NH$_3$ co-fueling and indirect engine cooling (system 6)

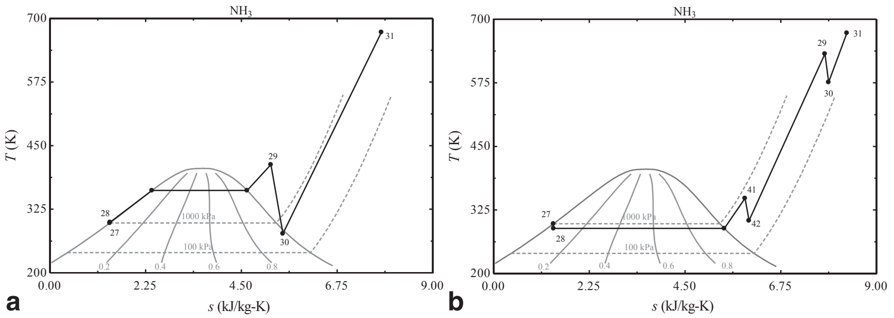

Fig. 8.25 *T-s* diagram of NH_3 recovery processes for **a** system 5, and **b** system 6

Table 8.4 NH_3 process results (system 5 and system 6).

Process	System 5	System 6
DSU heat recovery, $\dot{Q}_{DSU}$ (kW)	242	242
DSU product compression, $\dot{W}_{C2}$ (kW)	159.8	190
N_2 expansion work, $\dot{W}_{T2}$ (kW)	2.01	0.792
NH_3 expansion work, $\dot{W}_{T3}$ (kW)	58.75	38.7
NH_3 expansion work (system 6), $\dot{W}_{T4}$ (kW)	–	22.0

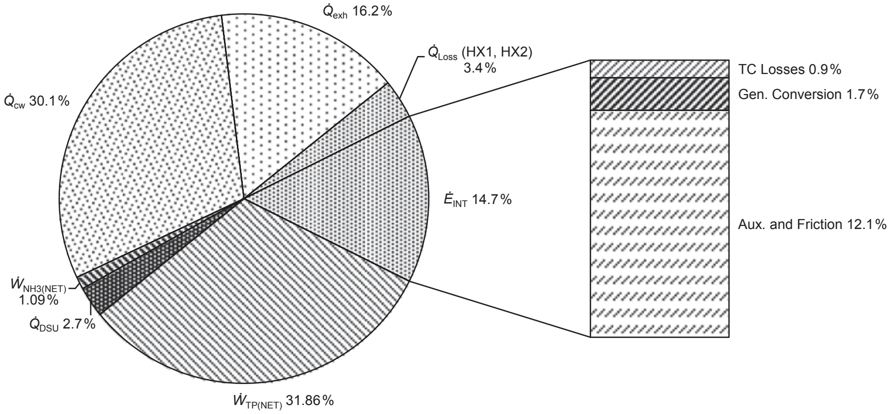

Fig. 8.26 System 5 energy balance ($\eta_5 = 0.345$)

Engine cooling (addressed in system 6) is a significant but necessary energy loss for the locomotive, and reducing the cooling load on the ICE by NH_3 indirect cooling can reduce the ICE power directed to water jacket and aftercooler processes. The energy balance for system 6 is shown in Fig. 8.28, and the energy efficiency is determined to be 34.2%. The exergy efficiency for system 6 is found to be 31.2%, with additional subsystem losses occurring in the second expansion process, due to turbine irreversibility and heat losses, shown in Fig. 8.29.

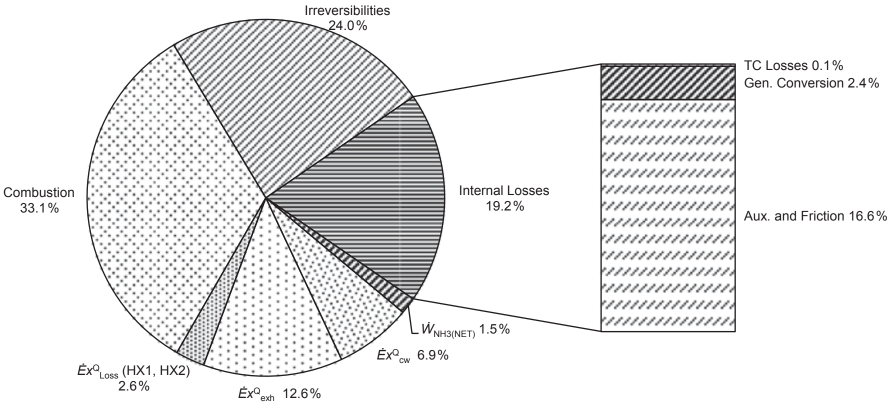

Fig. 8.27 Exergy destruction ratios for system 5 ($\psi_5 = 0.316$)

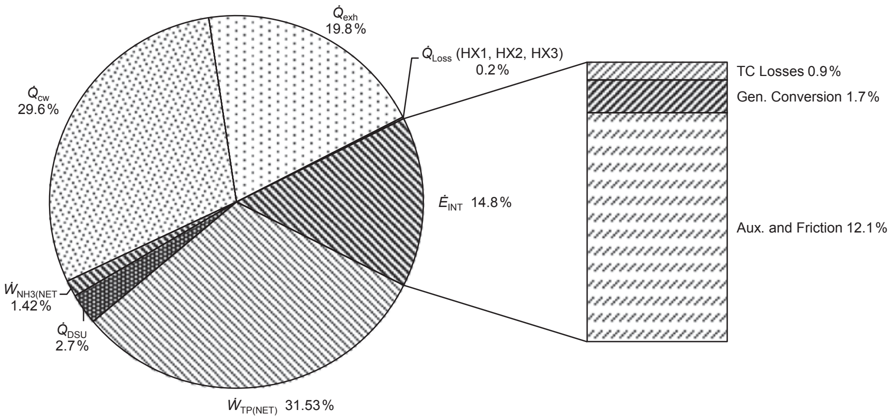

Fig. 8.28 System 6 energy balance ($\eta_6 = 0.342$)

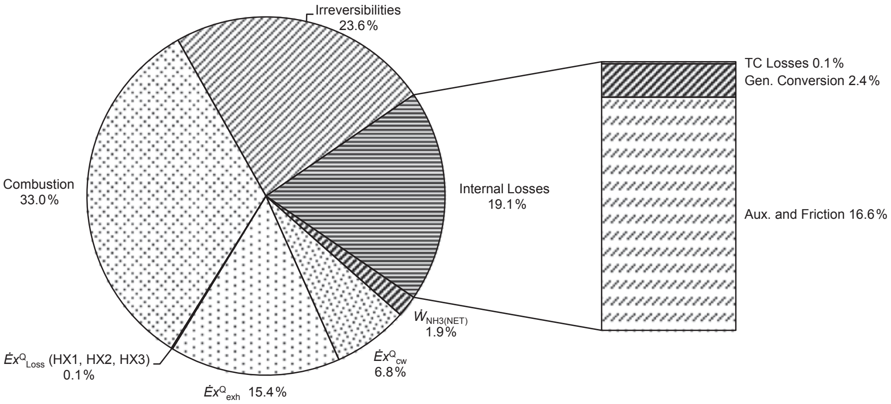

Fig. 8.29 Exergy destruction ratios for system 6 ($\psi_{60} = 0.312$)

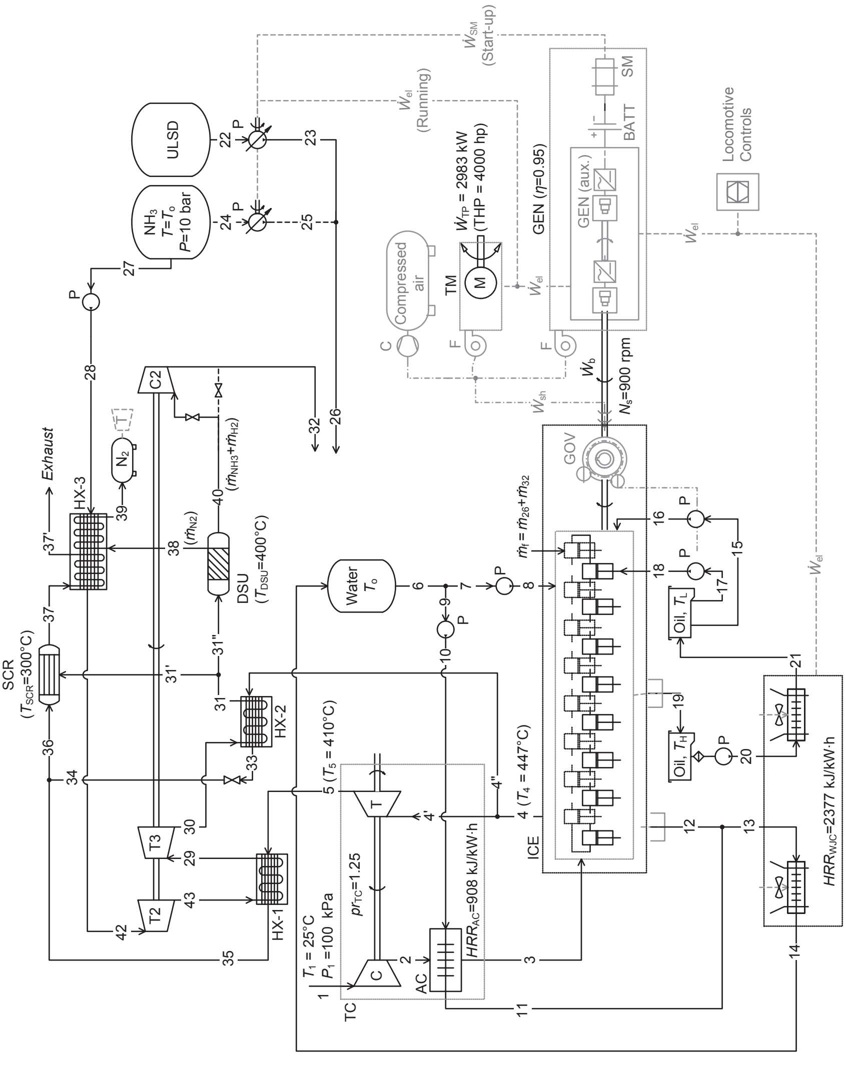

Fig. 8.30 NH$_3$ co-fueling and compressed N$_2$ gas storage (system 7)

Table 8.5 NH_3-process results (system 7)

Process	System 7
NH_3 pump, $\dot{W}_{P8}$ (kW)	0.852
DSU heat recovery, $\dot{Q}_{DSU}$ (kW)	242
NH_3 expansion work, $\dot{W}_{T2}$ (kW)	35.5
DSU product compression, $\dot{W}_{C2}$ (kW)	44.4
Compressed N_2 available work, $\dot{W}_{RES7}$ (kW)	1.104

The system configuration considered in system 7, and shown in Fig. 8.30, incorporates multistage NH_3 heat recovery and expansion, with the addition of compressed N_2 gas storage for on demand expansion work. The specific values for the work processes of the NH_3 subsystems are given in Table 8.5, and the NH_3 processes are shown in a *T*-*s* diagram shown in Fig. 8.31.

The available expansion work is considered as the isothermal work (Pv^n=constant; n=1), and an isentropic efficiency of 0.75. The compressed gas is stored at 500 kPa and atmospheric temperature. The heating of NH_3 for the first expansion in turbine T2 is obtained from the exhaust gases following the SCR process. The NH_3–H_2 and N_2 DSU product streams are cooled (not shown) before compression and storage, respectively. The energy efficiency for system 7 is determined to be 35.9 %, and the energy balance is shown in Fig. 8.32 for the ICE. The exergy efficiency for system 7 is determined to be 32.9 %, with the majority of NH_3 subsystem exergy destructions occurring in the heat exchange processes ratios are shown in Fig. 8.33.

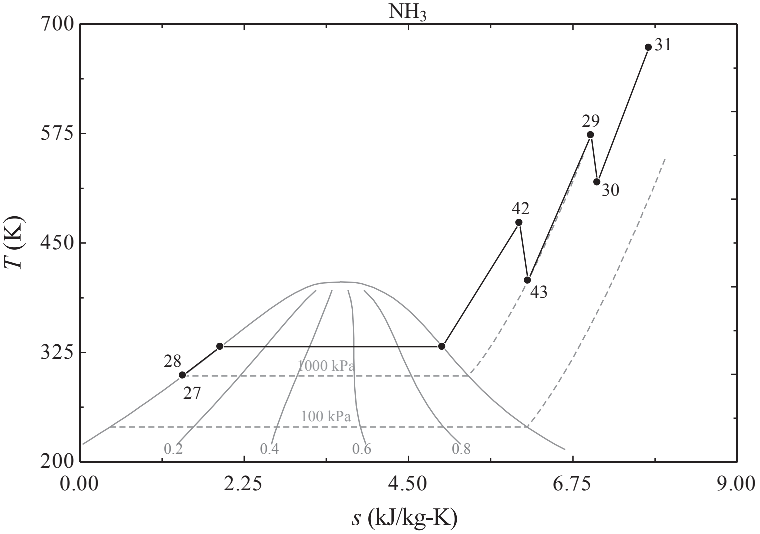

Fig. 8.31 *T*-*s* diagram of NH_3 recovery processes (system 7)

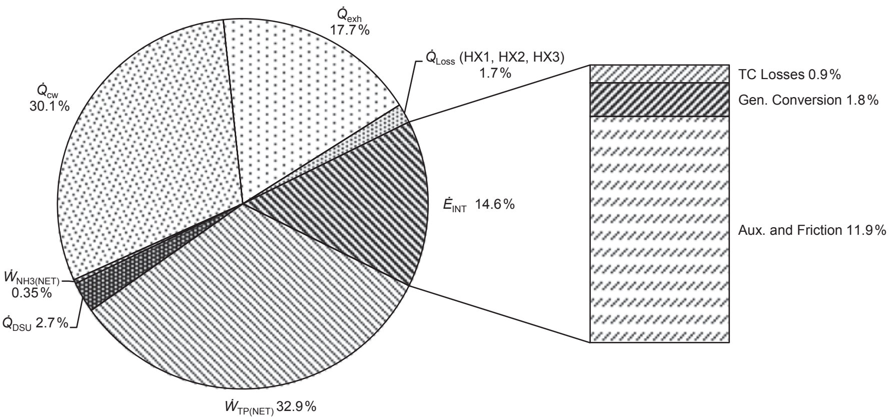

Fig. 8.32 System 7 energy balance ($\eta_7 = 0.359$)

Case Study III: Ammonia-Based Subsystem Integration Systems 8 and 9 provide cooling for the locomotive, using a turbine-driven fan in system 8, and a chiller (cooled by ammonia) for cab-cooling in system 9. The systems are shown in Figs. 8.34 and 8.35. Ammonia processes are shown in Figs. 8.36a and b for the systems.

In system 8, indirect engine cooling superheats the ammonia in HX3. The turbine is coupled by rotor to a fan that provides additional cooling to the radiator section, which further reduces the direct engine cooling by the ICE shaft work. System 9 provides cold storage, which is assumed to be applied to a cab air-conditioning unit at a coefficient of performance (COP) of 2.0, but could be applied to engine cooling, as well to potentially increase this effect. The system results for the useful work and heat products and the required work inputs are listed in Table 8.6 for each system.

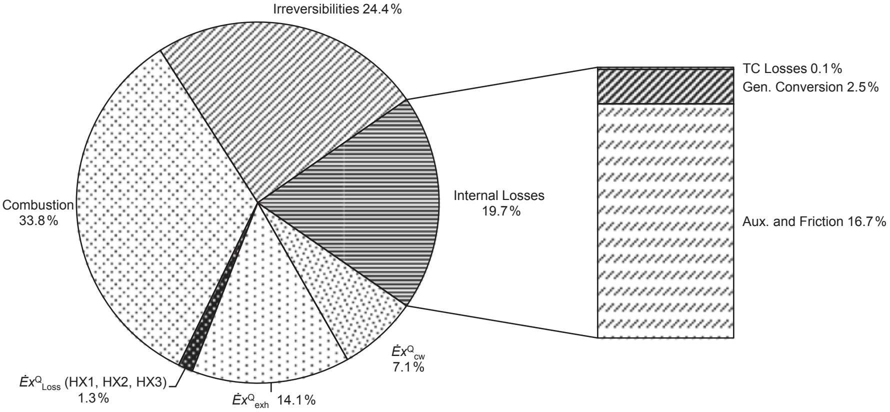

Fig. 8.33 Exergy destruction ratios for system 7 ($\psi_7 = 0.329$)

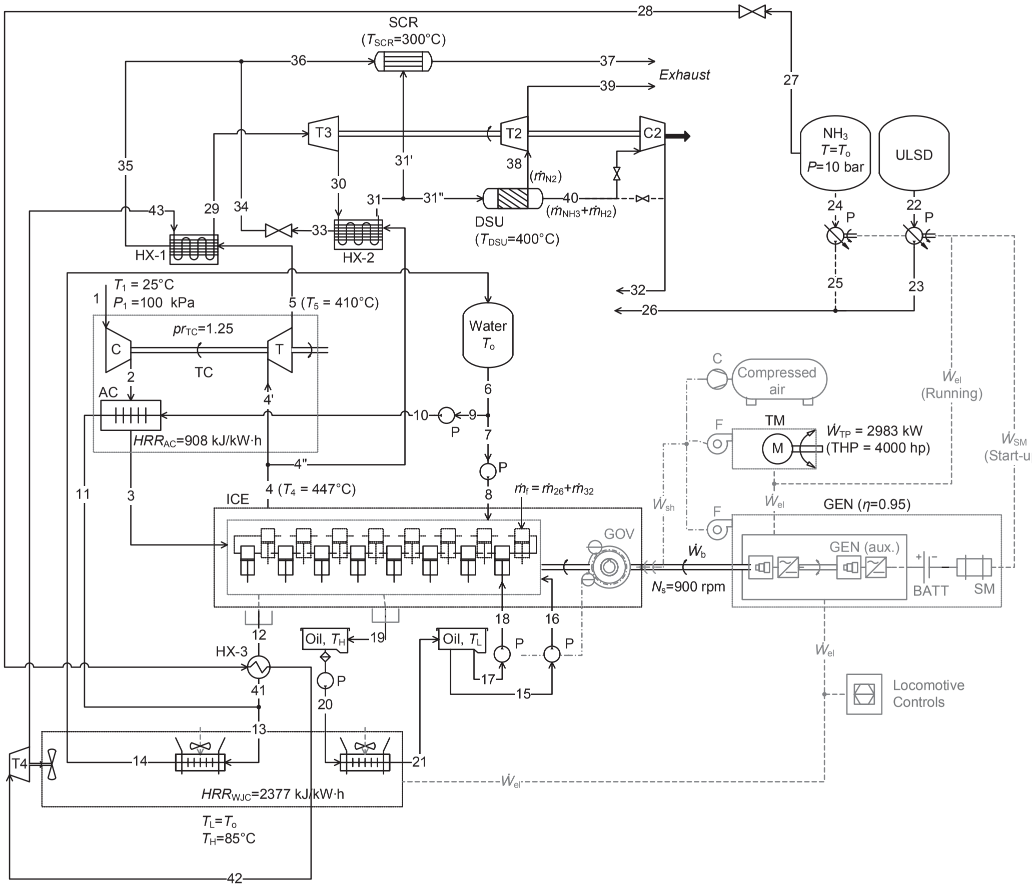

Fig. 8.34 NH$_3$ co-fueling and integrated fan cooling (system 8)

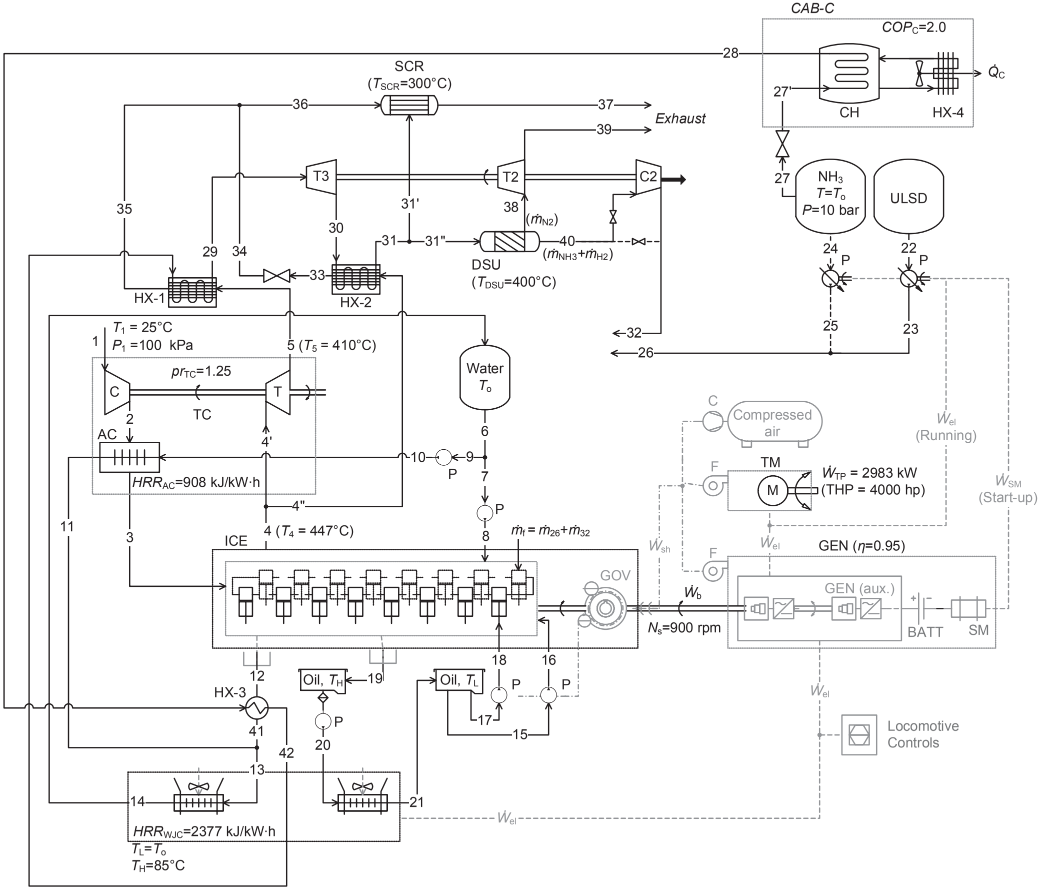

Fig. 8.35 NH_3 co-fueling and compressed N_2 gas storage (system 9)

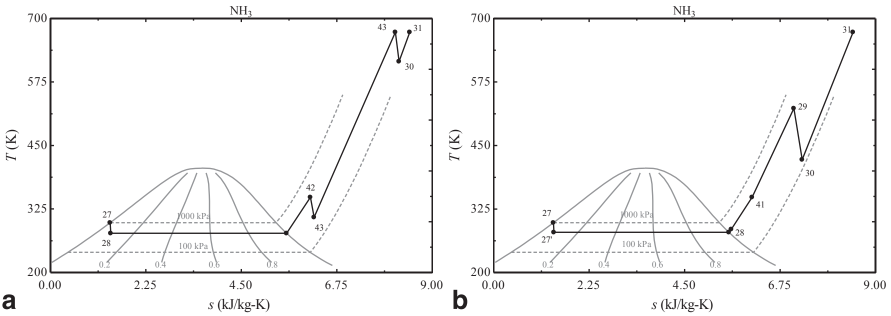

Fig. 8.36 *T-s* diagrams of NH_3 cooling and work processes for **a** system 8. **b** system 9

Table 8.6 NH_3-process results (system 8 and system 9)

Process	System 8	System 9
NH_3 indirect ICE cooling[a], $\dot{Q}_{\text{ICE-c}}$ (kW) (system 8)	112	–
Locomotive cab cooling, $\dot{Q}_{\text{CAB-c}}$ (kW) (system 9)	–	294
Cab cooling work input, $\dot{W}_{\text{CAB-c}}$ (kW) (system 9)	–	150
DSU heat recovery, $\dot{Q}_{\text{DSU}}$ (kW)	242	242
DSU product compression, $\dot{W}_{\text{C2}}$ (kW)	224	224
Expansion work, $\dot{W}_{\text{T2}} + \dot{W}_{\text{T3}}$ (kW)	41.7	0.318
NH_3 expansion work, $\dot{W}_{\text{T3}}$ (kW)	–	69.5

[a] System 8 indirect cooling by turbine driven fan $(Q_{\text{ICE-c}} = COP_c \cdot \dot{W}_{\text{T4}})$

The energy balance for system 8 is shown in Fig. 8.37, which has a calculated energy efficiency of 33.7 %. The heat recovery from the exhaust gases and coolant streams is used to generate turbine work both by removing heat from the fluids, and by driving a fan to provide forced air cooling. The heat recovered in the high-temperature heat exchangers at the exhaust is used to upgrade the temperature to the required DSU operating temperature.

The exergy efficiency for system 8 is determined to be 30.7 %, with the DSU product compression and higher temperature heat exchangers having the largest destruction ratios for the NH_3 processes. The exergy destructions for the system are shown in Fig. 8.38.

The energy balance for system 9 is shown in Fig. 8.39, which has an energy efficiency of 35.6 %. The system includes a locomotive cab-cooling subsystem that utilizes a chilled water tank to store cold-thermal energy produced by low-temperature NH_3 stream, which is throttled to lower pressure (and temperature) before entering the chiller tank. Liquid is circulated through a coil and a fan blows forced air over it, producing the cooling effect in the cab. The exergy efficiency for system 9 is calculated to be 30.9 %, with energy destructions described in Fig. 8.40.

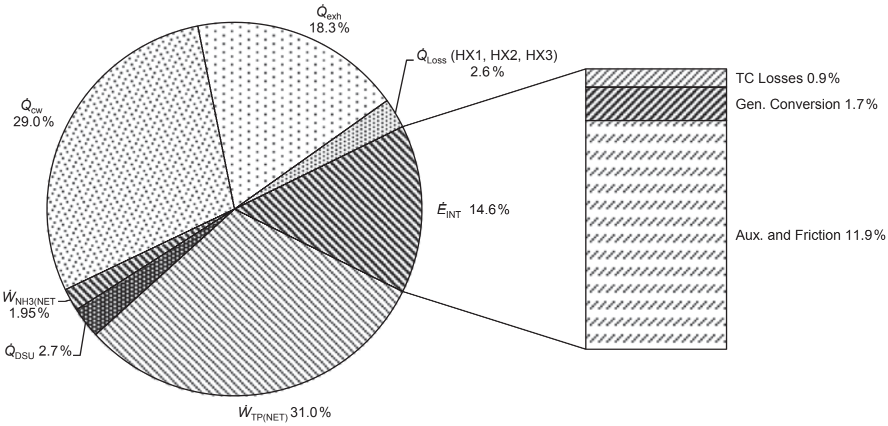

Fig. 8.37 System 8 energy balance ($\eta_8 = 0.337$)

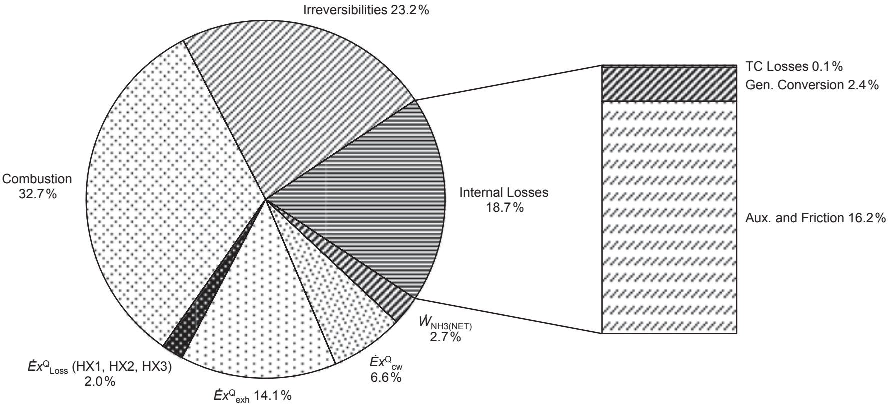

Fig. 8.38 Exergy destruction ratios for system 8 ($\psi_8 = 0.307$)

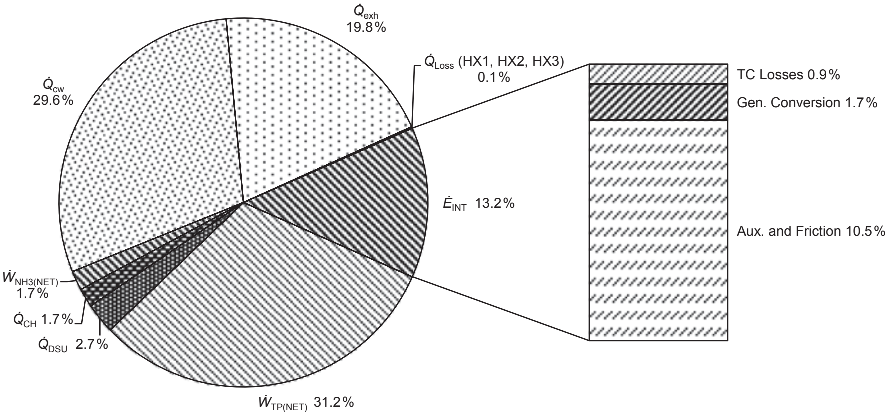

Fig. 8.39 System 9 energy balance ($\eta_9 = 0.356$)

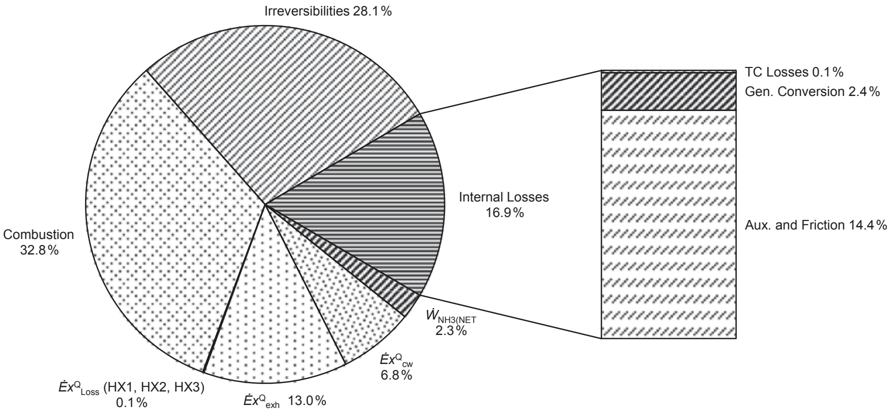

Fig. 8.40 Exergy destruction ratios for system 9 ($\psi_9 = 0.309$)

A cascaded approach is carried out in the exhaust heat recovery arrangement proposed for system 10 and the setup is shown in Fig. 8.41, where the waste heat from the ammonia Rankine cycle (NH_3-RC) used for process heating. The NH_3-RC operates in the same way as an organic Rankine cycle (ORC), which uses organic working fluids. The thermodynamic processes for the NH_3-RC and expansions are shown in Fig. 8.42. The operating principles used in the NH_3-RC are simple; saturated liquid NH_3 is pumped to an upper pressure level of 5000 kPa and then heated by exhaust waste heat to produce superheated vapor through a heat exchanger. The vapor is expanded in a turbine to produce shaft work. The low-pressure stream at the outlet rejects heat in a condenser and is recirculated as the cycle continues. By integrating an NH_3-RC, it is possible to take advantage of the higher pressure ratios, increasing the additional work produced from recovered heat in the NH_3-RC, as well as multi-stage expansion and reheat of the secondary ammonia stream. The NH_3-RC "boiler" uses exhaust waste heat after the SCR treatment, therefore, the high-grade exhaust heat in HX-1 and HX-2 is available for the additional heat recovery, and NH_3 expansion and decomposition processes.

The heat and work duties for the system are listed in Table 8.7. In the configuration shown in Fig. 8.41, the condensed ammonia stream is sent to the engine as fuel, but it may also be used in a closed circuit for the NH_3-RC.

System 10 has a calculated energy efficiency of 36.6 %, with the energy balance shown in Fig. 8.43. In this configuration, the heat recovery processes take an advantage of the different temperature levels available in the ICE heat losses. The NH_3-RC recovers heat from the exhaust after the SCR unit, and the high-temperature exhaust heat is used to produce expansion work by heating and reheating the NH_3 and to raise the temperature of the NH_3 stream to the DSU temperature. The exergy efficiency is calculated to be 33.5 % for system 10, with the exergy destruction ratios shown in Fig. 8.44.

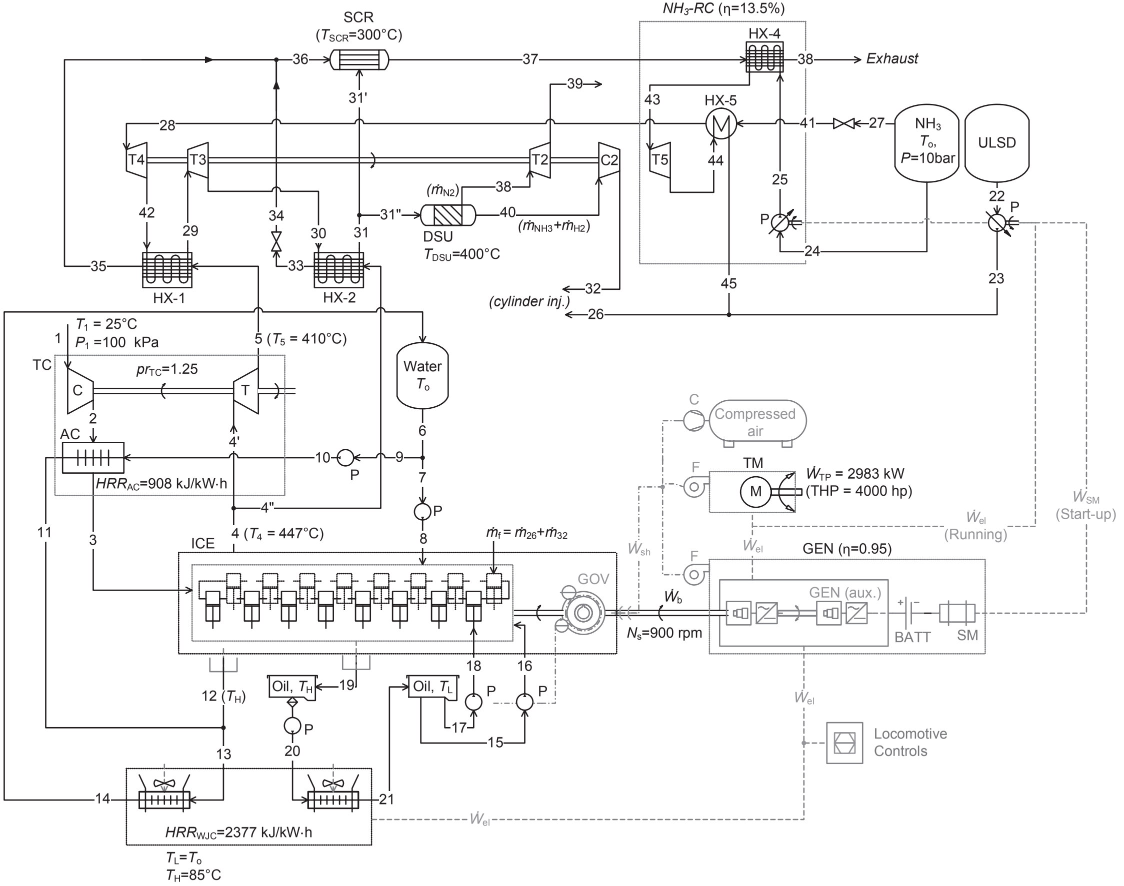

Fig. 8.41 NH_3 co-fueling and compressed N_2 gas storage (system 10)

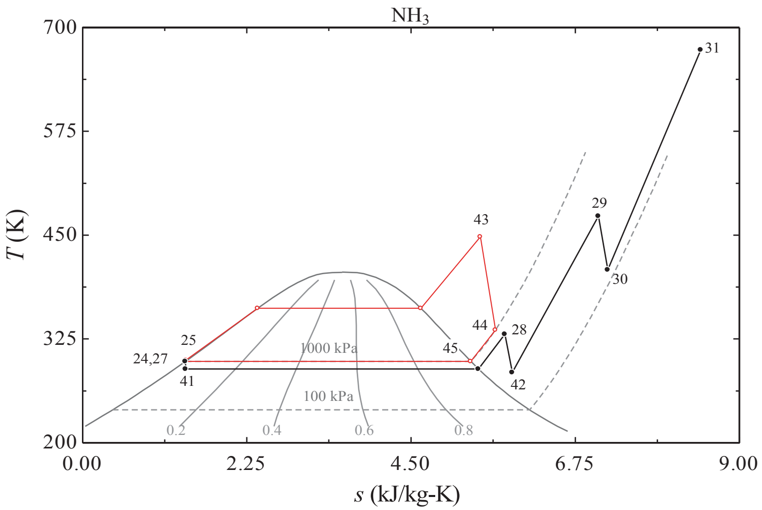

Fig. 8.42 *T-s* diagram of NH_3 recovery processes and integrated NH_3-RC (system 10)

8.5 Integrated Locomotive Systems Comparison

Energy and Exergy Efficiencies The effect on system performance by the ammonia-powered processes is evaluated based on of the heat recovery of the ammonia and additional work production determined in the system results. The results are shown in Fig. 8.45, comparing the utilization energy and exergy efficiencies achieved for each system at rated operating conditions.

Table 8.7 NH_3 process results (system 10)

Process	System 10
NH_3-RC pump, $\dot{W}_{P2}$ (kW)	2.27
NH_3 additional fuel pump, $\dot{W}_{P}$ (kW) (not shown)	2.39
NH_3-DSU return pump, $\dot{W}_{P}$ (kW) (not shown)	0.415
DSU heat recovery, $\dot{Q}_{DSU}$ (kW)	242
DSU product compression, $\dot{W}_{C2}$ (kW)	18.5
N_2 expansion work, $\dot{W}_{T2}$ (kW)	0.311
NH_3 expansion work, $\dot{W}_{T3}$ (kW)	38.4
NH_3 expansion work, $\dot{W}_{T4}$ (kW)	22.5
NH_3-RC expansion work, $\dot{W}_{T5}$ (kW)	50.8

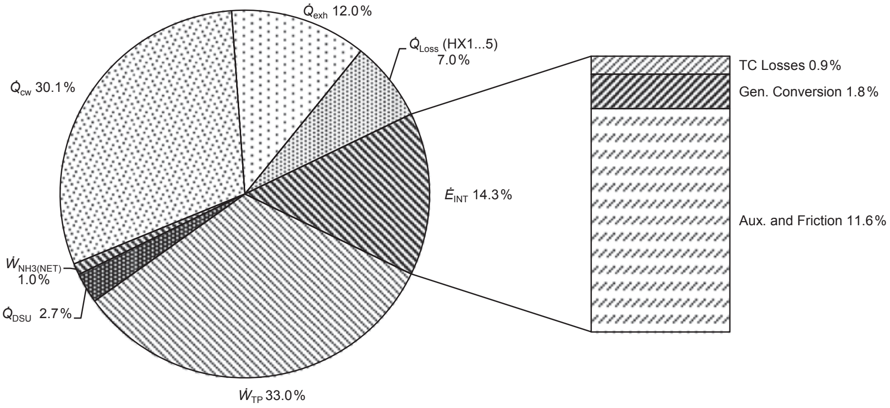

Fig. 8.43 System 10 energy balance ($\eta_{10} = 0.366$)

System 10 has the best performance both energetically and exergetically, and offers flexible operation in terms of generating capacity that can be increased by using a closed loop system instead of the flow-through scheme as described, which may supply additional power to the prime mover or the head end power system. The systems are investigated in greater detail in the following subsection with respect to the emissions produced by the selected fuel blend, overall sustainability, and the associated costs.

Environmental Impact

The following figures indicate the emission levels for the assumed fuel blend with 50% of fuel input from ammonia. The cases are shown for the CAC emissions, which are reduced by diesel reduction and by integration of the SCR unit (Figs. 8.46, 8.47).

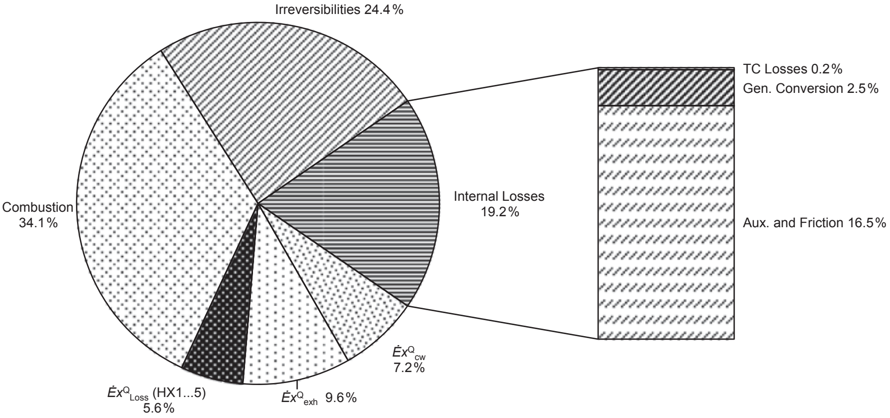

Fig. 8.44 Exergy destruction ratios for system 10 ($\psi_{10} = 0.335$)

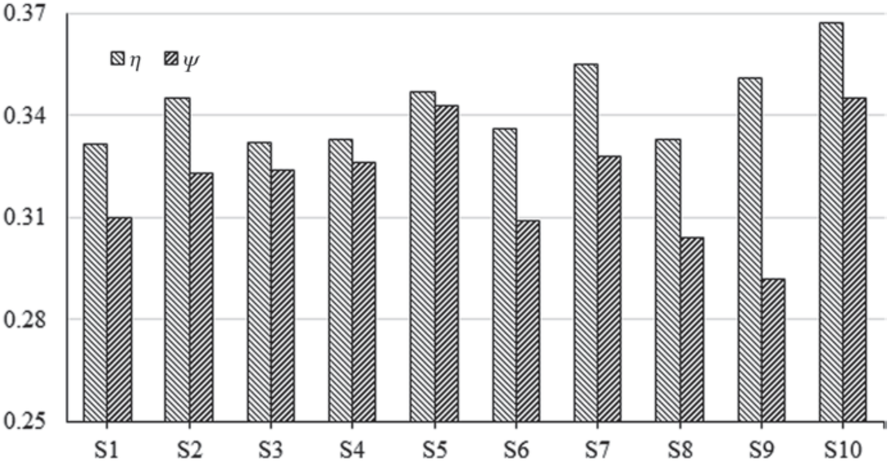

Fig. 8.45 Energy and exergy efficiencies for systems 1–10

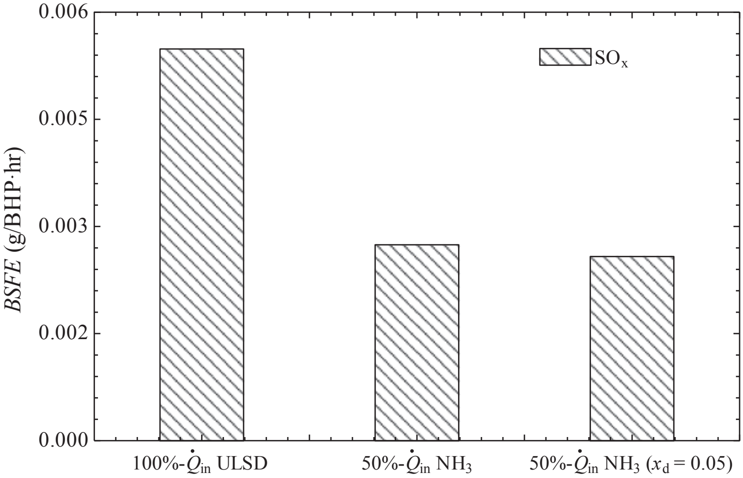

Fig. 8.46 SO_x emissions for fuel blends

Significant reductions for NO_x and HC emissions result with the SCR integration, with the lowest reductions observed for PM. Because ammonia contains no carbon, no soot is produced directly by NH_3 and, therefore, increasing the ammonia supply can help tofurther improve PM emissions (Figs. 8.48, 8.49, 8.50).

Capital Cost Estimation for Integrated Systems Estimated costs are outlined in Table 8.8 for additional equipment required for the proposed systems based on various cost data for similar equipment. The values are applied to each system to determine the change in system cost in Canadian dollars ($CDN_{\$2013}$) with a cost index.

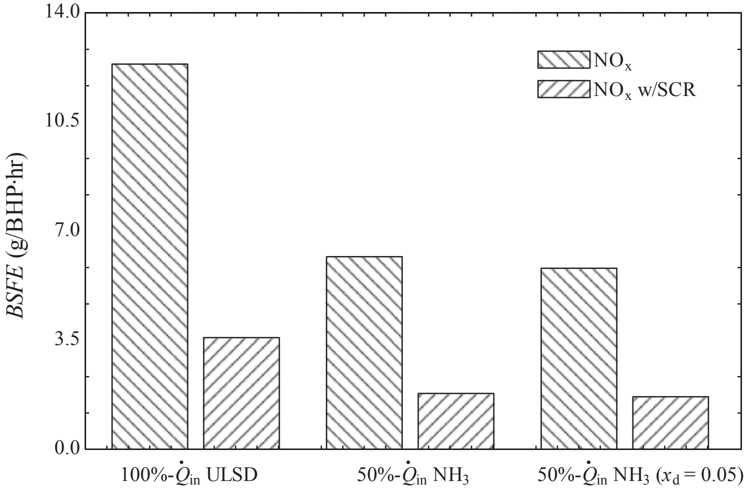

Fig. 8.47 NO_x emissions and SCR reduction for fuel blends

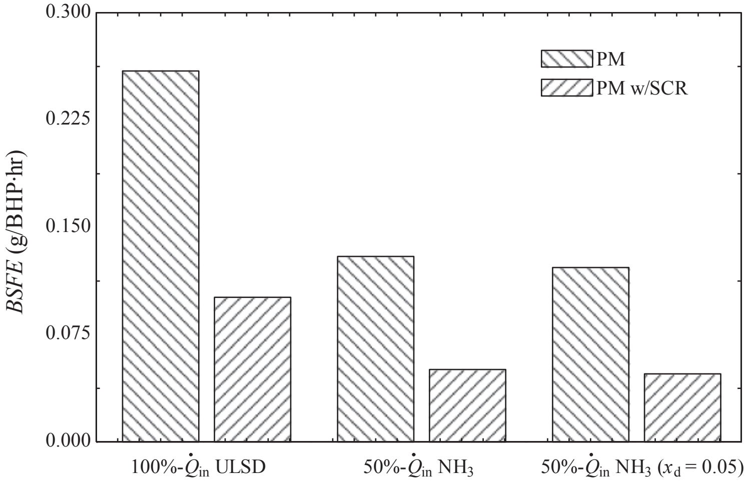

Fig. 8.48 PM Emissions and SCR reduction for fuel blends

The estimated total costs for each system are listed in Table 8.9 based on the reference base costs and component capacities for each of the systems. These estimates give a baseline for comparison, even though a more rigorous system cost analysis should be conducted in subsequent design stages with greater detail.

Sustainability Assessment Results The Greenization factor (GF) for each fuel blend is shown in Fig. 8.51, with constant factors resulting for systems 3–10 based on the assigned fuel mixtures. The maximum reduction is calculated to be 53 %, or a GF of 0.53.

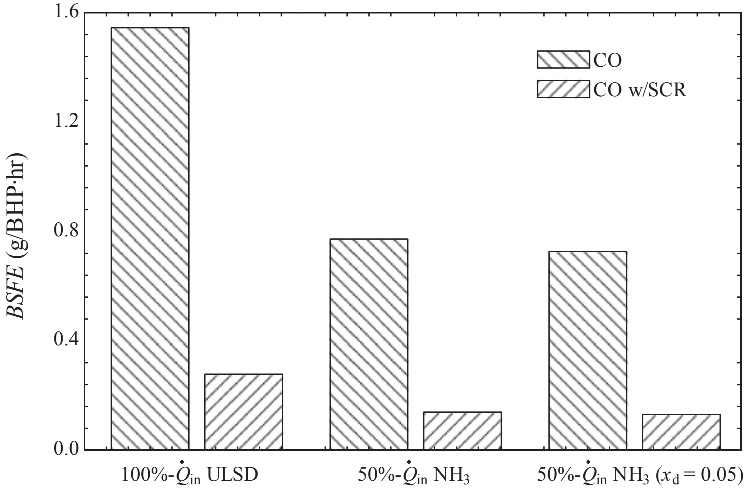

Fig. 8.49 CO Emissions and SCR reduction for fuel blends

The depletion factors are shown in Fig. 8.52. These results give a clear indication of the performance in terms of the amount of exergy destroyed. From the results shown, systems 8 and 9 have significant losses that make these less attractive and as a potential option; however, because the energy is recovered from waste heat, these options still have value if the desired products are met—specifically, cabin air cooling and supplementary engine cooling. systems 5 and 10 have the lowest depletion factors and make an efficient use of the recovered energy.

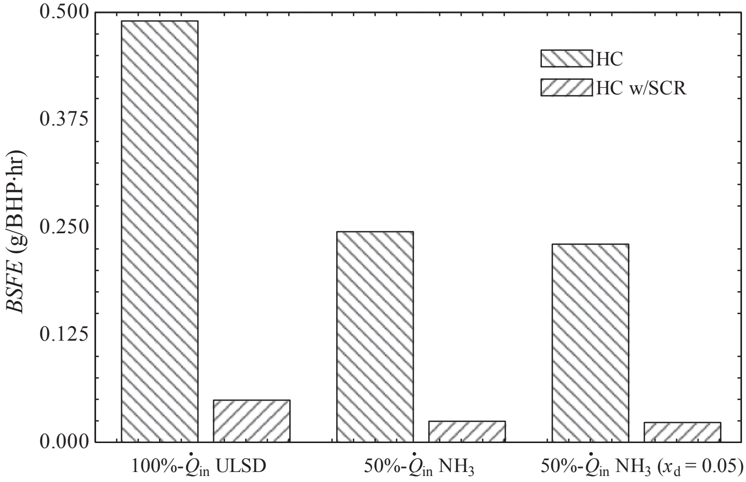

Fig. 8.50 HC Emissions and SCR reduction for fuel blends

Table 8.8 Estimated capital costs of additional equipment. (Sources: [105, 111–114])

Equipment item	Reference cost data	
	C_0 (USD$_{year}$)	S_0
SCR system	150,000\$$_{2003}$	2.0 MW$_{TP}$
NH_3 DSU	275\$$_{2007}$	1.0 kW$_{H2}$
Dual-fuel conversion	250,000\$$_{2003}$	(per unit)
NH_3 pressure storage tank	1,450\$$_{2006}$	1.0 m^3
Pump	400\$$_{2006}$	1.0 kW
Gas compressor	25,000\$$_{2006}$	100 kW
Gas compressor	2000\$$_{2006}$	2.25 kW
Power recovery turbine	10,000\$$_{2006}$	40 kW
Air conditioning unit	60,000\$$_{2006}$	700 kW$_{th}$
Exhaust recovery heat exchanger	55,000\$$_{2007}$	300 kW$_{th}$
ORC unit	70,000\$$_{2007}$	20 kW h
Fan	8250\$$_{2006}$	60 kW h

Table 8.9 Estimated total capital costs of additional equipment for locomotive systems

System	CDN$_{\$2013}$
System 1 (SCR only)	398,090
System 2	720,860
System 3	1,030,960
System 4	1,032,035
System 5	1,039,700
System 6	1,092,075
System 7	1,051,210
System 8	1,085,450
System 9	1,077,800
System 10	1,144,090

The increase in total cost of the locomotive is evaluated based on the capital cost estimated for the required system equipment for each configuration. The system "S1" is the only case where the SCR technology is being implemented with no additional ammonia processes. Overall, the majority of the systems are found to have capital cost that increases, ranging 10–15 % from the base locomotive cost (Fig. 8.53).

System Comparison To evaluate the overall system performance, considering all the performance factors, the assessment results are compared using a target plot. Following the methodology by [115], the results for each impact factor are normalized to rank the systems highlight and the best case, which is shown in Fig. 8.54 within the black outer circles. For the factors that concern the fuel mixture—GF

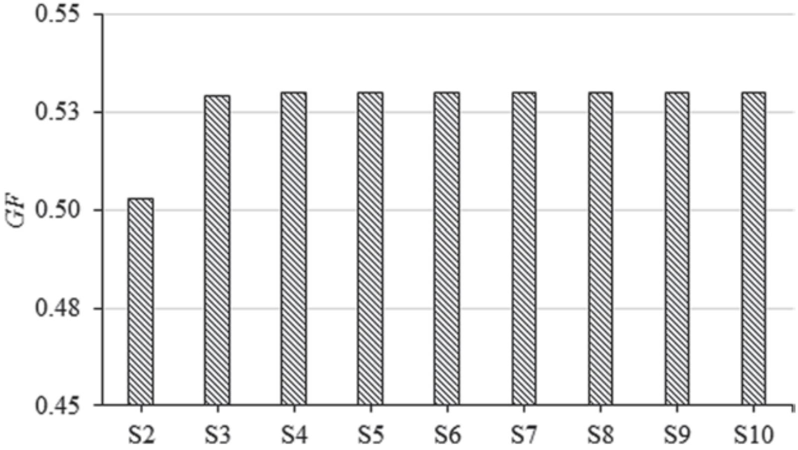

Fig. 8.51 Greenization factor *(GF)* for systems 2–10 (S1 = 0)

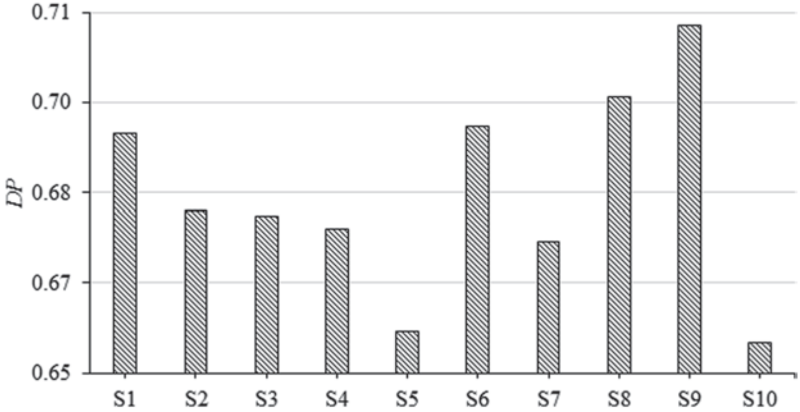

Fig. 8.52 Depletion factor (D_P) for systems 1–10

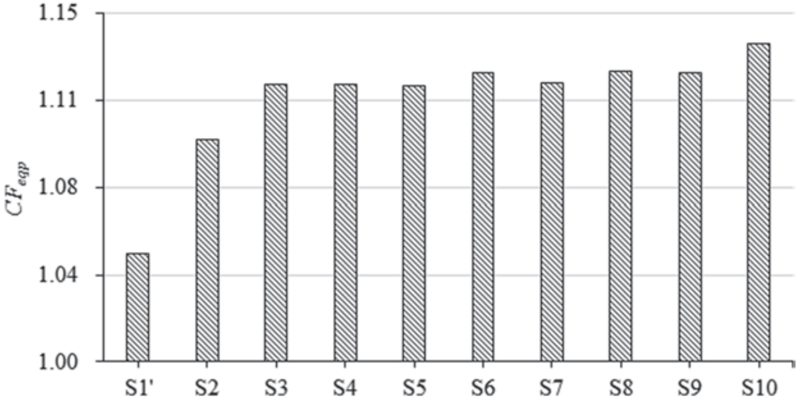

Fig. 8.53 Relative cost increase for additional equipment

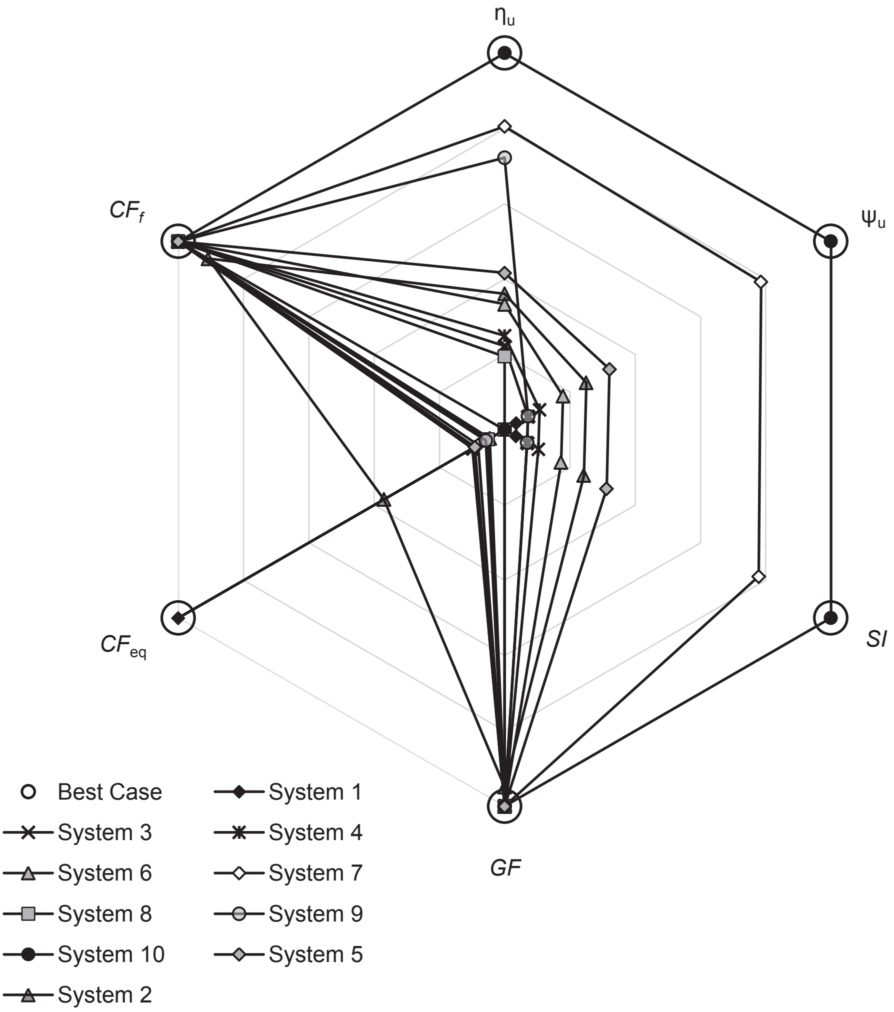

Fig. 8.54 System comparison

and CFf—the rankings show the associated systems grouped by either diesel-only (system 1), NH3 diesel (system 2), and NH3–H2 diesel (systems 3–10). The plotted results not only show that system 10 performs the best in terms of its efficiency and has the highest sustainability index, but also shows that these advantages come at the highest cost for the additional equipment.

Different cases are considered in Fig. 8.55 to represent the system comparisons with the significance given to a particular performance factor. These prioritized factors represent decision-making scenarios—for example, green initiatives or cost savings in fuel—are highlighted by applying weight factors to the performance results. The weight factor represents the priority consideration. In the first case as

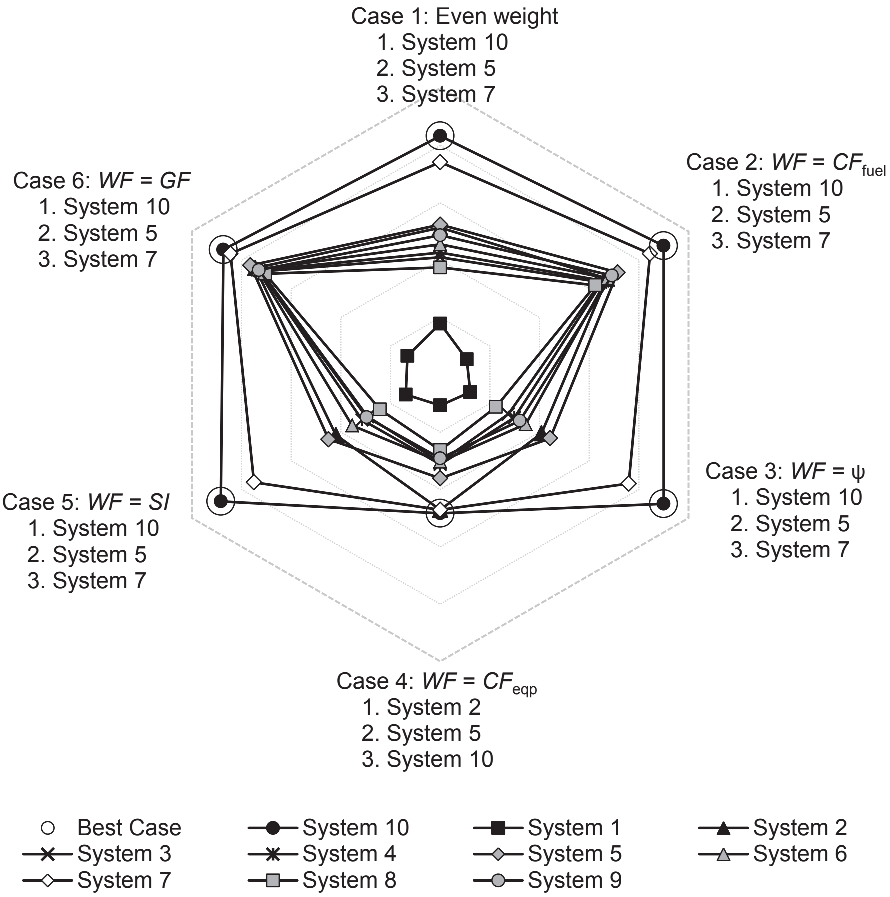

Fig. 8.55 System comparison with weighted factors

shown in the figure, even the weight is given to each factor considered, including the Sustainability Index, fuel cost factor, equipment cost factor, Greenization factor, and the energy and exergy efficiencies for each system. Weighting factor cases 2–6 highlight the different factors as a priority to show the influence of that aspect of system performance within the overall assessment.

The results are summarized briefly in Table 8.10 for systems 10, 5, and 7, which rank the highest for their overall performance for the given comparison. These systems appear to be the best options and are good candidates for demonstration. While the systems are investigated based on the operating conditions of a specific locomotive, included components and subsystem processes are generally scalable and may be optimized based on the operating conditions specific to various locomotive engines.

Table 8.10 Summarized results for the top three ranked systems

	System 10	System 5	System 7
Description	NH_3-RC multistage heat recovery and expansions	Multistage heat recovery and expansions	Multistage heat recovery and N_2 compressed gas storage
Energy efficiency, η (%)	36.6	34.3	35.9
Exergy efficiency, ψ (%)	33.5	31.5	32.9
Greenization factor (GF)	0.53	0.53	0.53
Estimated equipment cost, C_{eqp}, CAD_{2013}	$1,144,086.00	$1,039,700.00	$1,051,700.00

8.6 Illustrative Example: GO Transit Commuter Rail in the GTA

The GO rail system is one of the Canada's largest commuter rail networks, handling 185,000 passengers on weekdays, using 47 locomotives. The GO Rail commuter fleet includes 65 tier-2 emission compliant, MP40PH-3C diesel-electric locomotives, capable of pulling/pushing 12 bilevel passenger coaches. The transit system operating details are given in Table 8.11. Ammonia fueling is considered for use in GO Rail operations, and the potential of the ammonia fueling is addressed for the overall fuel cost and environmental performance.

The duty cycle operation is given in Table 8.12 for commuter operation, with the daily operating time combined for notch 1 (N1) and dynamic braking (DB). Duty cycle average GHG emissions per passenger and cost of the fuel for weekday commuter operation of the GTA GO rail transit system are determined for the baseline diesel-fueled case, and the considered ULSD-NH_3–H_2 fuel blend with 50% energy input by NH_3, and NH_3-decomposition of $x_d = 0.05$ to produce H_2 fuel.

Fuel prices are assumed to be 1.24 CDN$/L for diesel fuel and price range for ammonia to be 400–700 CDN$/tonne-$NH_3$ (0.24–0.42 CDN$/L), accounting for the effect of significant price fluctuation of natural gas on ammonia cost. The results are given in Table 8.13 for ammonia co-fueling in the rated notch position (notch 8), which has the exhaust emission temperatures high enough to maintain the system operation as described and the highest fuel consumption, and the remaining notch

Table 8.11 GO transit commuter rail details. (Source: [32])

Passengers (weekday)	185,000
Number of lines	7
Stations	63
Route kilometres	450
Weekday train trips	203
Weekday train-sets in use	47
Locomotives (MP40PH-3C, tier 2)	65
Bi-level passenger coaches	563 (162 seats)
Fuel capacity	8410 L

Table 8.12 Locomotive duty cycle for commuter rail transit [20]

Engine notch	Low idle	N1, DB	N2	N3	N4	N5	N6	N7	N8
RPM	200	269	343	490	568	651	729	820	904
% Daily operating time	59	6.1	2.3	2.2	2.1	1.3	1.2	1.8	24
Average power (kW)	15	150	300	745	1044	1342	2480	2610	2983

Table 8.13 Duty cycle fuel consumption and fuel cost for GO Rail MP40 locomotive (ULSD-NH_3–H_2 blend used in notch 8 only (idle and notch 1–7 use 100 % ULSD)

	100 % ULSD	50 % Q_{in} NH_3 (x_d=0.05 H_2 production)	
		ULSD	NH_3
Fuel mass consumed per duty cycle (kg)	2857	1693	2625
Volume consumed per duty cycle (L)	3360.00	1992	4353
Combustion GHG emissions (kg-CO_2)	8950	5305	–
Combustion GHG's per passenger (kg-CO_2/PAX)	2.05	1.14	
Fuel cost per duty cycle (CDN$)	~$4166	$2,470	$1050–1838
Total fuel cost per duty cycle (CDN$)	~$4166	$3520–4308	
CO_2-tax ($15/ton-$CO_2$)	$134	$30	–
Total with imposed CO_2-tax (CDN$)	$4300	$3550–4338	

positions fueled by diesel fuel. The emissions per passenger do not include the emissions produced when the locomotive is in low idle and idle (N1) notch positions, to better represent the commuter case when the locomotive is in transit.

The calculated results show that there is a potential significant economic benefit to use the fuel blend; with a 15 % fuel cost reduction for fuel blending used in notch 8 with lower NH_3 price, but it becomes less competitive if the cost of natural gas increases. Encouraging the production of ammonia from renewable resources may help to lower the average cost by creating price competition with natural gas production, as well as improving the environmental performance of ammonia for the total lifecycle. Combustion GHG emissions are significantly reduced, with results indicating a 44 % reduction in combustion CO_2 emissions per passenger.

8.7 Closing Remarks

This chapter investigates the use of ammonia as a combustion fuel, heat transfer fluid, NO_x-reducing agent, hydrogen resource, and working fluid in a locomotive application. Ten systems are included in the comparative assessment, developed with long-term sustainability and environmental impact reduction as the primary aim. While the current methods to produce ammonia are associated with some GHG emissions, it may be produced from any renewable resource and is able to provide significant cost and environmental impact reductions.

From the comparative assessment, the following conclusions are made with respect to the system performance:

- From a sustainability standpoint, system 10 has the best performance, followed by system 5 and system 7.
- In terms of emissions, the NH_3 systems all perform well with significant reduction in GHG and CAC emissions by SCR reduction, and diesel fuel replacement by ammonia.
- With respect to the cost performance, although the systems appear to have poor performance when compared to the original system (without additional systems) this is due to capital costs. With the lower cost of ammonia and with more competitive renewable technologies, the operational costs will reduce over time.

With the reduction of large emission sources and improvement of railway infrastructure, it is possible to make more reasonable estimations of the potential improvements by ammonia systems on rail performance. Advanced data logging and tracking techniques along with detailed modeling studies have a potential to present more insight to railway transportation sector's emissions.

- Different methods of sustainable ammonia production should be investigated to reduce the lifecycle impact of ammonia fuel.
- Further research should be conducted on developing cheap and efficient fuel purification, cleaning, and storage systems.
- Advanced fuel technologies should be developed and investigated to optimize the mass and volume requirements, system efficiency, emissions, as well as the system cost for onboard hydrogen production at different capacities from ammonia.
- System design improvement studies including weight and volume reduction should be conducted to reduce the space demand in the locomotive.
- In addition to the aforementioned technical recommendations, further research should be conducted on how to gain public awareness for ammonia.
- System scalability should be further investigated to provide solutions for light duty vehicles.

Chapter 9
Concluding Remarks

Nowadays, the world depends on non-sustainable resources as an option for energy supply. Owing to this reason, the transportation sector worldwide is not sustainable. The main reason of this fact is the stringent discrepancy between fossil fuel cycle and the natural cycles in the ecosystem. Mineral fuels extracted massively are burned in power plants, converted in refineries, and combusted in transportation vehicles everywhere, resulting in the emission of greenhouse gases (GHG) and other pollutants that affect the ecosystem. Negative environmental impact due to anthropogenic activity does not delay to manifest in the form of global warming, soil and water acidification, ozone layer depletion, etc.

The transportation sector is obviously responsible for large amounts of GHG emissions. Within this sector, a good deal is due to the operation of diesel electric locomotives, but also due to the operation of electric locomotives that require power, as much of the power is produced in a non-environmentally benign manner. In face of this situation, many jurisdictions and private and public institutions are alarmed and they are responding to the situation by taking various initiatives.

In this book, the clean rail transportation options are reviewed. In order to review the options clearly, the major ecological problems related to the anthropogenic activity are presented in Chap. 1. The growth of the population comes together with the desire of people for a better standard of life; this leads to higher demands of commodities, of which, the energy and transportation demand stands at the high point. Of course, the rail transportation, covering freight and passenger transport has a determinate role in promoting clean practices. Therefore, the conventional practices and the potential clean rail solutions are discussed here in detail.

The quick methods toward a cleaner rail transport involve the application of aftertreatment methods and biodiesel blends. Although easy to apply, these practices have some downsides. Biodiesel fuel is not sufficiently tested for long-term operation. In particular, there are technical issues with the fuel durability in the context when the railway needs to store and manipulate large amounts of fuels. Regarding the aftertreatment, the most difficult to apply is the selective catalytic reduction (SCR), for which the technology is not yet commercially developed in the railway

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sector. The SCR system is massive and requires huge maintenance. As an example, in an application, a special tender railcar is used to carry a properly sized aftertreatment unit including scrubbers.

Probably, a ready-to-apply solution is the use of a methanol-based railway transportation. Provided that the carbon dioxide is extracted from the atmosphere and hydrogen is produced from renewable sources, this solution becomes perfectly sustainable, as it integrates with the water and carbon dioxide natural cycles. However, the today's technology does not permit a fully sustainable methanol transportation. Although technically possible, a huge investment is required for making the methanol locomotive an actual solution. Renewable hydrogen and carbon dioxide extraction from the ecosystem are also not considered as developed technologies.

Nevertheless, methanol railway can be implemented today, although not in a fully sustainable manner, by removing carbon dioxide at emission sites (power plants, cement and metallurgical plants, and other stationary combustion plants), and then using it to generate methanol to drive locomotives. This solution brings environmental benefits with no doubts and also prepares the world for better sustainability in the future.

Another ready-to-apply solution is the ammonia-based railway. The fully sustainable option of this imposes an integration of ammonia fuel cycle with the water and nitrogen natural cycles. This is possible with the present day technology, although scaled-up research is required for the development of direct ammonia fuel cell technology and ammonia internal combustion engines. As discussed in the book, this option does not pose any technological barriers. In view of this perspective, the book insists on ammonia-based railway options.

Nine novel systems are presented in the book and assessed in detail for specific case studies that deal specifically with ammonia as energy source. Ammonia is a very promising substance used for transportation, with interesting properties. First ammonia is a fuel by itself and it can combust with air, producing only steam and nitrogen (theoretically). Second, ammonia is an NO_x reducing agent, meaning that, when properly designed, an ammonia engine will reduce its own NO_x emissions. Third, ammonia can be used as a hydrogen source by itself and can be decomposed easily into hydrogen and nitrogen. This means that ammonia can produce its own combustion promoter—the hydrogen—in a tunable proportion according to the momentary needs of the engine. Furthermore, ammonia can be directly used in direct ammonia fuel cells, a proven technology in course of scaling-up nowadays. Fourth, ammonia is an excellent refrigerant, and therefore it can be used for cooling the engine and, if the engine is properly designed, it can be used for cooling the cabin. Finally, ammonia can be used to some extent as a working fluid to generate power by expansion.

All these features of ammonia are explained in this book by the systems presented in the case studies. In order to comparatively assess the systems, the core thermodynamic methods are briefly introduced, using energy and exergy concepts. Furthermore, the economic and environmental assessment methods are presented. The use of these methods allows a thorough and meaningful comparative assessment of the newly proposed systems with respect to a reference baseline system.

Besides the ammonia systems—the focus of the book—other emerging system are discussed to some extent, one of them is the hydrogen locomotive. Significant research programs were initiated by various institution and jurisdictions around the world and are mentioned in the book. Hydrogen offers some good deal of flexibility with respect to fuel production and fuel utilization. For instance, hydrogen can be used both in internal combustion engines and in fuel cells to drive locomotives. Also, there are various potential and commercially viable methods to generate hydrogen. The main drawback of hydrogen as fuel is related to its storage problem. Hydrogen is difficult to store and distribute because it is difficult to compress in its pure form. In addition, there is no available method to generate sustainable hydrogen using only renewable (or nuclear) energy. Due to this reason, the current technology is not capable of integrating the hydrogen fuel cycle within the natural water cycle of the ecosystem. This implies that widespread use of hydrogen-based rail transport is a far away projection for the future, as technologies become more mature and available.

As a promising option, the natural gas railway locomotive is also mentioned in this book. Most likely, liquefied natural gas (LNG) locomotive is to be developed. The technology is already demonstrated to convert diesel electric locomotives to LNG carried in tender railcars. This technology is readily applicable as demonstrated by full-scale projects in the USA and Canada. There is room for development though for better efficiency. In this regard, as mentioned in this book, solid oxide fuel cells with integrated methane reforming and gas turbine are highly promising for railway locomotives. The emissions of LNG railway locomotive are not only significantly lower than the diesel electric one but also are lower than that of the electric locomotive when the power generation emissions are taken into account. Therefore, it is suggested that LNG railway locomotive is a ready-to-apply option for a cleaner global railway transportation. Nevertheless, all solutions have their appealing advantage, and in this perspective, the ammonia-based rail transport brings probably the best integration potential with the natural ecosystem.

Due to the growth of freight and passenger traffic, less time is available for the maintenance. In the future, it is expected that infrastructure maintenance costs will decrease significantly because of the fact that there is an increasing interest toward the development of new control and materials technologies, which will require less maintenance. There will also be implementation of new developed technologies. Furthermore, the installation of automatic inspection and maintenance techniques will deliver enhanced capacity while increasing safety and security. Safety and security aspects of rail transport are treated carefully, and new technologies are potentially available to address these. This, together with improved processes and methodologies, will boost passenger and freight attractiveness.

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