A NEW SIMPLE INDEX FOR THE ESTIMATION
OF ENERGY IMPACTS ON THE ENVIRONMENT

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Abstract

A new methodology is presented for relating the generation and/or the consumption of heat and electrical energy to the rate of CO_2, NO_2, and SO_2 emissions to the environment. Two indices are provided for the precise determination of emissions of these gases to the atmosphere and are of help in the analysis and comparison of the quality and efficiency of energy options. The indices have no linear dependency on energy consumptions (unlike EIA and EPA methodologies) and can be applied to any industry in which heat or electricity is used. The new methodology requires minimal data, such as fossil fuel characteristics and heat flow through heaters and electrical energy consumption by fans, pumps, and compressors. Two case studies are provided to illustrate how the new methodology quantifies such emissions and how the technique can be employed in screening alternative technologies or designs.

Key words: climate change, energy consumption, energy efficiency index, exergy, impact assessment

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1. Introduction

Climate change, acid rain, global warming and the emissions of pollutants are of great concern to scientists, engineers, environmentalists, governments and today's society at large. The rationale behind this concern includes the improvement of human and animal health, awareness of threats to people and the preservation of a clean environment and natural resources for the next generation, saving money and resources, and above all respecting national laws and policies. A number of different attempts have been made to analyze the production of waste materials in order to reduce their effect on the environment, which is discussed in more details in the succeeding section.

Although the existing methods have several advantages which make them applicable in a variety of situations, they have also few disadvantages such as inaccuracies or restricted applications to buildings and so forth. The generation of energy from fossil fuels such as coal, natural gas and oil has an adverse effect on the environment due to the formation of gaseous pollutants (Department of Environment, Food and Rural Affairs, 2013; EPA, 1997; Suteu et al., 2016).

Industrial operations such as chemical manufacturing complexes and fossil-fueled power plants have a considerable interest in finding a simple and accurate relationship between energy generation and gas pollutant emissions to the atmosphere, a subject also of concern to environmentalists and regulators. Such a relationship may encourage regulators to develop programs stimulating the protecting of the environment from gaseous emissions. Industrial investors are restricted by environmental regulations, such as the cataloguing and disposal of chemical wastes and the cost impact of the exposure of chemical and hazardous wastes to the environment. For them to devise and implement

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strategies for pollution prevention, incentives such as tax reduction, subsidies, and loans or credits for the on-site recycling of wastes, and research and development assistance will be certainly necessary (Cohen and Giralt, 1996; Schiopu et al., 2007).

Many researchers, engineers and environmentalists use the annual reports of the Energy Information Administration (EIA) or the US Environmental Protection Agency (EPA) to relate the energy generated or consumed by manufacturing industries and power plants to their CO_2 emissions to the atmosphere. The present paper offers an alternative methodology, relating thermal or electrical energy (in kJ/h) to CO_2, NO_2, and SO_2 emissions to the environment in kg/h, based on the characteristics of the fossil fuel employed for the generation of heat and power (EPA, 1997; Suteu et al., 2016).

The new methodology provides a simple index for estimating the emission rate of gas pollutants when the heat or power consumption is known, for example from the nameplate of electric motors. Chemical manufacturing industries are concerned with energy consumption in the following ways:

   - boilers for steam generation to initiate and accelerate chemical reactions, to heat reboilers, and to generate electricity;
   - cooling towers for removing heat from reactors, coolers, condensers etc.
   - electric power for running rotary equipment such as pumps, fans, compressors, blowers, agitators etc.

Coal, natural gas and oil are the main fossil fuels having relatively high energy content. The combustion of fossil fuels results in gaseous emissions to the atmosphere such as CO_2, NOx and SOx. In steam turbine power plants the energy of the steam is transformed into electricity. The conversion efficiency of a steam turbine is 35% (EPA, 1997) and that of a boiler is 75% (Coulson and Richardson, 2001).

The generation of heat and electricity on the plant scale requires technically sophisticated equipment and high expenditure, and at the same time depleting natural energy resources. The more effective the use of electricity or steam within industry, the more environmentally friendly the process becomes and the better the preservation of global natural energy resources.

2. Materials and methods

Important methodologies have been established for the estimation of the energy impact of a given process on the environment. These are discussed in the next three subsections. In the fourth subsection we will introduce the proposed new energy index and summarize its benefits.

2.1. The EPA methodology

The EPA has developed standalone software for the evaluation of the impact of materials and energy on the environment, known as WAR GUI

(2008). This program is based on a waste reduction (WAR) algorithm for the estimation of the potential environmental impact (PEI) of a chemical process. The PEI theory is an amendment to the WAR algorithm. It employs eight environmental impact categories, including global warming, ozone depletion and acidification potential, for the assessment of the impact of a chemical substance on the environment (Young et al., 2000).

The impact of energy discharge on the environment is reported in PEI/h by WAR GUI (2008). The methodology is based on the available air emission data for fossil fuel electric power generation from coal, oil or gas. These data are collected from the energy and waste inventories of utility and non-utility electricity generation plants. These data may be classified into a range of categories based on industry size, geographic distribution of utilities and non-utilities, their capacity by prime movers, fossil fuel energy source (i.e. gas, coal or oil), type of producer (e.g. small power producer, or co-generator), waste and pollutant generation, waste release profile, emissions to the atmosphere, annual air pollutant releases, emission factors for gas-fired, coal-fired and oil-fired power generators, inorganic and organic hazardous air pollutant (HAP) emissions etc.

The EPA method (WAR GUI, 2008) provides impact rates for each type of fossil fuel expressed in PEI per unit energy for each impact category. This is multiplied by the energy generated in the plants in unit energy per hour to give the energy impact expressed as PEI per hour. The assumption made by the EPA to validate this calculation is that the rate of pollution emission is directly dependent on the amount of energy required (WAR GUI Tutorial, 2008). Table 1 presents the impact of four sample categories in PEI /MJ for different types of fossil fuel.

Table 1. The impact rates for each fossil fuel (PEI/MJ) for each impact category (WAR GUI Tutorial, 2008)

Category	Coal	Gas	Oil
HTPI [a]	7.83E-05	4.76E-08	9.14E-05
GWP [b]	1.93E-04	9.57E-05	1.52E-04
ODP [c]	2.03E-09	3.63E-10	0.00E+00
AP [d]	5.98E-03	9.92E-04	3.74E-03

[a]*Human toxicity potential by ingestion;* [b]*Global warming potential;* [c] *Ozone depletion potential;* [d]*Acidification potential*

The EPA (2013) has also provided conversion factors for the estimation of CO_2 emissions, ranging from electricity consumption to vehicle fuels, as well as the combustion of natural gas, oil, coal, etc. The factor for the fossil fuel conversion might be expressed in the following form: *7.0555×10^{-4} metric tons CO_2 / kWh, or 196 mg CO_2/kJ.*

The above method provides no information about other gas emissions such as NO_2 or SO_2. There is also a significant difference between this method and that of the EIA even though both are interconnected governmental organizations, which is discussed in the following section.

2.2. Energy Information Administration (EIA) data

The EIA is a US governmental organization which prepares annual reports for energy consumption from both clean and fossil fuel sources, as well as pollution emissions in a number of countries around the world. Using the EIA data, boiler or turbine efficiency factors are not applied.

The energy content of a fuel can be roughly calculated when the total fuel consumption and generation of CO_2 are known. The necessary data are available from the EIA. For example, the following data for fossil fuel energy consumption and CO_2 emissions in Canada during 2006 have been obtained from the EIA website (EIA, 2009):

- Total energy consumption: 13.9×10^{15} BTU (oil, 32%; hydro, 25%; natural gas, 24%; nuclear, 7%; coal, 10%; other renewable, 1%).
- Energy-related carbon dioxide emissions: 614×10^6 tonnes.

The overall contribution of fossil fuels to energy consumption is about 66%. Other sources of energy include solar, nuclear, hydro, etc., which are regarded as clean energy sources and therefore make no contribution to CO_2 emissions. The total carbon dioxide emissions reported above by the EIA are thus derived solely from fossil fuels and can be related to energy consumption in kJ in the following relationship (Eq. 1):

(614 × 106 tons CO₂/13.95 × 1015 × 0.66 BTU) × (1.055 kJ/ BTU) × (106 g/tonne) = 63 mg CO₂/ kJ)
$$(1)$$

Hence, 1 kJ energy consumption in the form of heat or electricity releases 63 mg CO_2 as an environmental pollutant. This method, however, gives only a ball-park figure for CO_2 emission to the atmosphere. It also has two other disadvantages:

(1) the EIA methodology does not reveal the contribution of fossil fuel types to CO_2 emissions;

(2) the data for NO_X and SO_X emissions are unavailable. Therefore no relationships can be established between emissions from a particular fossil fuel (e.g. oil, gas or coal) and energy consumption.

There is a significant difference between this method and the EPA method in Section 2.1, above.

3. Other methodologies

3.1. Exergy methodology

In thermodynamics the term *exergy* is defined simply as (Yantovski, 2004) the maximum available useful work, and is derived by Eq. (2):

$$A = \Delta U - T_o\, \Delta S + P_o\, \Delta V = \Delta\,(U - T_o\, S + P_o\, V) \quad (2)$$

The term *A* was originally denoted availability or available energy, but since 1956 it has come to be described as exergy. ΔU is the difference in internal energy, $T_o\, \Delta S$ is the entropy loss or heat loss, and $P_o\, \Delta V$ is the available *PV* work. Unlike energy, which changes from one form to another, exergy is irreversible and is destroyed in a closed system due to friction and the increase in entropy according to the Second Law of Thermodynamics. The exergy is expressed in the explicit form as given by Eq. (3) (Fan and Zhang, 2012):

[Partial molar exergy at T and P, $\bar{\varepsilon}$] = [Partial molar chemical exergy, $\bar{\varepsilon}_0$] + [Partial molar thermal exergy, $\bar{\varepsilon}_T$] + [Partial molar pressure exergy, $\bar{\varepsilon}_P$]
$$(3)$$

and in mathematical form (Eq. 4):

$$\bar{\varepsilon} = \bar{\varepsilon}_0 + \int_{T_0}^{T} \overline{C_p}\,(1 - T_0/T\,)dT + \int_{P_0}^{P}\left[\overline{V} - (T - T_0\,)\left(\partial V/\partial T\right)_P\right]dP$$
$$(4)$$

where $\bar{\varepsilon}_0$ is the partial molar chemical exergy (kcal/gmol) and is to be found in thermodynamic handbooks; for instance $\bar{\varepsilon}_0$ for water in the liquid and gaseous states are 0 and 56.23 kcal/gmol, respectively.

Exergy is employed for the evaluation of sustainable design performance by estimation of the design efficiency. Its applications include building lighting, cooling and ventilation, and home electrical appliances (Canadian Architects, 2012).

The efficiency is defined by Eq. (5):

$$\eta = \frac{available\ energy\ transfer\ of\ the\ desired\ kind\ achieved\ by\ the\ system}{available\ energy\ input\ int\ o\ the\ system}$$
$$(5)$$

Although the concept of exergy has provided improvements in sustainable design, it gives neither information on the impact of energy on the environment nor is it widely applied to chemical processes but in initial stage of industrial application (Luis and van der Bruggen, 2014).

3.2. Ricardo - AEA

The Carbon Trust (2013) has provided a fact sheet containing a number of conversion factors for carbon emissions from different energy sources within business and public energy consumption. These factors are based on the annual interactive report published on the UK Government website of the Department of Environment, Food and Rural Affairs (2013).

The conversion factors are calculated on the basis of both user's requirements including year, energy type such as fuel (natural gas, CNG, LNG, LPG, solid fuel), bioenergy, passenger vehicle, UK electricity etc., type of requested report, greenhouse gas (CO_2) and so on as well as Ricardo–AEA factor (2013). The user can select the fuel type from the website:

http://www.ukconversionfactorscarbonsmart.co.uk/Filter.aspx?year=27.

A list of questions then will appear which have to be answered correctly to start calculations, followed

by clicking on download button. An Excel file will open when the calculation is completed. For fuel oil the net calorific value (CV) in 2013 was 40.70 GJ/tonne fuel oil (compared to natural gas, 47.73).

The database is collected on an inventory basis and is therefore subject to change each year; for instance, the net CV for fuel oil in 2012 was 40.72 GJ/tonne and fell by 0.02 GJ/tonne the following year. Although this website provides a number of conversion factors for transportation, fossil fuel and biofuel consumption, it provides no relationship between heat flow and gas emissions.

3.3. Energy Usage Index (EUI)

The EUI is a methodology used for calculation of energy consumption within premises in BTU per unit area. The corresponding database can be downloaded from the website of the Oregon Department of Energy (2013). EUI requires the following data for calculation:

1.   12-month utility bills,
2.   Square footage of the premises, and
3.   Hours of operation.

An example of the EUI is the School Interactive Database (SID), in which the above data are entered in the spreadsheet and the energy consumption in BTU/sq ft is calculated. Unfortunately, this methodology cannot be used for chemical process plants.

3.4. Energy Index calculation

Software has been developed by Texas Instruments (2013) for calculating the energy index of building per unit temperature per unit area, e.g. BTU/sq ft, degree day (BTUDD); the lower the index the more energy efficient are the premises. As in the case of EUI, this index is beyond the scope of the present paper.

3.5. Energy Efficiency Index (ODEX)

The energy efficiency index (ODEX) (EEA, 2012) is related to 10 industrial categories; chemical, steel, paper, non-ferrous, cement, food, machinery, transport equipment, textile and other non-metallic. The ODEX is a weighted average of the contribution of each category to the total energy consumption in a given year. In the first three industries the specific consumption per tonne of production is used, and for the remainder the ratio of energy consumption to the production index is employed.

This methodology deals only with energy savings in specific industries*, and may be useful for operating companies as it needs actual energy consumptions and savings over a period of time (several years) but not in design phase.* In addition, it gives no information about gas emissions to the atmosphere.

3.6. Energy Development Index (EDI)

The IEA (International Energy Agency, 2012) has presented four indicators for the evaluation of the energy function in human development as a tool to help estimate the UNDP's (United Nations Development Programme) Human Development Index:

• per capita commercial energy consumption as an indicator of a country's economic development;
• per capita electricity consumption in residential zones;
• the contribution of modern fuels in the total residential area;
• the proportion of the population without access to electricity.

Eq. (6) is used for calculation of the above indicators to track a country's transition toward the use of modern fuels:

$$Indicator = \frac{Actual\,Value - Minimum\,Value}{Maximum\,Value - Minimum\,Value} \qquad (6)$$

The World Energy Outlook publishes annually the Energy Development Index (EDI) for the international awareness and monitoring of the progress of individual countries from energy poverty towards modern energy access.

3.7. Energy Efficiency Design Index (EEDI)

The energy efficiency design index (EEDI) is a complex index developed by Germanischer Lloyd SE (2013) for application to improvement of the energy efficiency of ships and other maritime activities. *The complex EEDI method calculates* CO_2 emissions and is a function of the type of ship and fuel, and specific fuel oil consumption by main and auxiliary engines and power take-off devices, such as shaft generators, propulsion power etc. *EEDI is a long mathematical model and a number of parameters to be estimated and this is why the model is not provided here. And finally the EEDI is defined as* (Eq. 7):

$$EEDI = \frac{CO_2\ Emission}{Transport\ Work} \qquad (7)$$

3.8. Energy Performance Index (EPI)

The energy performance index is the ratio of annual primary energy consumption to aggregate product output (http://www.seai.ie/Your_Business/Large_Energy_Users/Special_Initiatives/Special_Working_Groups/Commercial_Buildings_Special_Working_Group_Spin_I/Commercial_Buildings_Benchmarking_Irish_Context.pdf). Any change in energy performance therefore results in a change in the EPI. EPI is calculated by Eq. (8):

$$EPI = \frac{Energy}{Output} \times F \qquad (8)$$

where F is a factor used to set the *EPI* to 100 for the first year the company joins the program. This allows F to be set for succeeding years. As an example, for an energy usage of 2,500 GWh and production output 100, F equals to 4 (Eq. 9):

$$F = \frac{Output}{Energy} \times EPI = 4 \qquad (9)$$

For subsequent years, for energy usage of 2,750 GWh and output 112 the EPI becomes 98.21, and so on. In practice EPI is expressed as a five-page report containing the primary energy per unit of output and estimated CO_2 emissions, and the relationship changes with emissions with energy performance. The total CO_2 emissions in the current year are then calculated based on the fuel type and the electricity consumption in GWh, and then multiplied by the EPI difference between current and earlier years. For instance, typical data for heavy fuel oil (HFO) might be as follows:

- HFO consumption   47.04 GWh
- Conversion   274
- CO_2 emissions   12,888.876 tonnes

The conversion factor for HFO is thus 274 tonnes CO_2 emissions/GWh, or 76 mg/kJ. The general conversion factor from EIA is 63 mg/kJ (refer to Eq. 1) The existing methods encompass several disadvantages leading to inaccurate results. For example, both EPA and EIA methods provide no information about NO_X and SO_X gas emissions. Besides, the EIA methodology does not reveal the contribution of fossil fuel types to CO_2 emissions. The exergy methodology neither gives information on the impact of energy on the environment nor is it widely applicable to chemical process design phase. Ricardo–AEA provides no relationship between heat flow and gas emissions.

Both Energy Usage Index & Energy Index calculation may be used for buildings but not for chemical process plants. ODEX is useful for operating plant and needs detailed operation data over few years. In addition, it gives no information about gas emissions to the atmosphere. Energy Development Index (EDI) is an indicator to monitor the progress of individual countries from energy poverty towards modern energy access. The energy efficiency design index (EEDI) is a complex index for the improvement of the energy efficiency of ships and other maritime activities and needs detailed information about the fuel, engine and propeller. The energy performance index (EPI) is the ratio of annual primary energy consumption to aggregate product output. EPI needs detailed operational data from company's energy consumptions and product output over a range of years. Hence, there is still a widely demand to a simple and quantitative index to be preferably applicable (but not limited) to the initial stage of the process design at minimum available data. The new indices will establish a relationship between the heat flow (and/or energy consumption) in a chemical process and the rate of CO_2, SO_2, NO_2 emissions to the atmosphere (as the impacts of energy generation and consumption on the environment).

4. Proposed new energy impact index

This paper offers a new methodology to establish a direct relationship between the energy produced from fossil fuels in the form of heat or electrical power to the polluting gas emissions, e.g. CO_2, NO_2 and SO_2. This relationship can be accurately established using the stoichiometry of the combustion of carbon, nitrogen and sulfur atoms using:

(a) the chemical composition of the fuel,
(b) the enthalpy of combustion of fossil fuels,
(c) the heat content of the fuel.

The advantages of this new methodology are as follows:

- the calculation can be made using minimal available data;
- the methodology can be used at an early stage of process design, despite lack of detailed process data. It can also be used in an operating plant for the estimation of emission rates based on energy consumption by pumps, compressors etc.;
- unlike the EPA and EIA methods, there is no need to determine the flow rate of fuel;
- the method can be extended to non-process applications in which heat or electricity is generated or consumed by or from fossil fuels;
- it provides detailed information about process units, chemical or petrochemical complexes, and fossil-fueled power plants in terms of environmental acceptability.

When the objective is the estimation of rate of CO_2 emission by the combustion of a fuel, assuming the combustion efficiency equals to unity, the Eq. (10) can be employed:

$$\dot{I}_e = \frac{(\dot{Q} \times x_C \times MW_{CO_2})}{(\Delta H_{Comb.} \times MW_C)} \qquad (10)$$

where $\dot{Q}$ is the heat flow (kcal/h), x_c is the mass fraction of carbon component in the fuel, MW_{CO2} and MW_C are the molecular weights of carbon dioxide (kg CO_2/kg mole) and carbon atom (kg C/kg mole), respectively, and $\Delta H_{Comb.}$ is the enthalpy of fuel combustion (kcal/kg fuel), and $\dot{I}_e$ is the emission rate of carbon dioxide to the atmosphere in kg CO_2/h.

In practical applications in which a hydrocarbon fuel is burned, ΔH_{Comb} is replaced by *HV* (Annamalai and Puri, 2002), the heat value of the fuel (Eq. 11):

$$HV = -\Delta H_{Comb} \qquad (11)$$

In the course of fuel combustion water is generated. Depending on the state of the produced

water, the heat value is defined as the lower heat value (LHV) for the gaseous water phase and the higher (or gross) heat value (HHV) for the liquid aqueous phase (Eqs. 12, 13):

$$LHV = \Delta H_{React.} - \Delta H_{Prod., H2O\,(g)} \qquad (12)$$

$$HHV = \Delta H_{React.} - \Delta H_{Prod., H2O\,(l)} \qquad (13)$$

Thus, replacing ΔH_{Comb} by the heat value (HV), followed by rearrangement of Eq. (10), the Eqs. (14) to (16) are obtained:

$$\dot{I}_e = \sum_j \dot{I}_j \qquad (14)$$

$$\dot{I}_{j,k} = \sum_i x_i \times \left(\frac{\dot{Q}_{i,k}}{\eta_k \times HV}\right) \times \left(\frac{MW_j}{MW_i}\right) \qquad (15)$$

$$\dot{I}_j = \sum_k \sum_i \dot{I}_{j,k} = \sum_k \sum_i x_i \times \left(\frac{\dot{Q}_{i,k}}{\eta_k \times HV}\right) \times \left(\frac{MW_j}{MW_i}\right) \qquad (16)$$

In the above equations, η is the efficiency; k is a process unit (e.g. fired heater, heater, and electromotor). For instance, when the estimation of the emission due to electricity consumption by a compressor is of interest, in this case k is an electromotor and η_k is the total efficiency, given by the multiplication product of the conversion efficiencies of boiler and steam turbine. $\dot{Q}_{i,k}$ is the fraction of the heat flow and/or the energy consumption related to component i (kcal/h), where i = C, S and N, in process unit k. HV is the heat value of the fuel (kcal/kg fuel), x_i is the mass fraction of component i, and MW is its molecular weight (kg/kgmole). The subscripts i denotes the atom content of the fuel (i = C, S or N) and j denotes the gas emitted to the atmosphere (j = CO₂, SO₂, NO₂). $\dot{I}_{j,k}$ is the gas emission rate to the atmosphere in the form of component j due to either heat or electricity consumption in the process unit k in kg CO_2 (or SO_2 or NO_2) per hour.

In Eq. (16), it is assumed that each atom contributes to the heat flow or the energy generation based on its mass fraction in the fossil fuel. This assumption is valid, since the heat flow is a size-dependent property, which means that the fuel heat flow depends on the flow rate of individual components in the fuel. In other words, the heat flow is the sum of the heat released by combustion of each component of the fuel, and doubling the flow rate of each component of the fuel doubles the corresponding heat flow. Depending on the nitrogen to oxygen ratio, oxidation of nitrogen gives two distinct products; a 7:8 ratio gives nitric oxide (NO) and a 7:16 ratio gives nitrogen dioxide (NO₂) (McMurray and Fay, 2003). Similarly, the burning of fossil fuels containing sulfur releases SO₂ into the atmosphere. While SO₂ is slowly oxidized to SO₃ by oxygen in the atmosphere, on the large scale this reaction can be catalyzed by V₂O₅ and in the presence of heat and water produces sulfuric acid. Both SO₂ and SO₃ are known to give rise to acid rain, a major environmental issue (McMurray and Fay, 2003). Hence, in the present paper it is assumed that the combustion reactions conducted in the presence of excess air and that the nitrogen and sulfur content in a fossil fuel is each converted to the most stable form (NO₂ and SO₂, respectively).

Since hydrogen and water are not regarded as pollutants, neither of these is of interest in terms of gaseous emissions. It is very important to recognize that in a chemical process plant, gas emissions related to energy consumption such as electric motors does not necessarily take place in the plant location itself, but may occur in power plants or co-generation plants in which fossil fuels are burned to generate heat or electricity. Steam turbine plants using fossil fuels account for the greatest proportion (more than 42%) of industrial applications. Among other fossil fuels gas provides the best energy source, since it generates fewest pollutants, at the same time requiring few handling facilities such as piping or storage tanks (EPA, 1997). A study has shown that the emission of CO₂ from fossil fuels gave the highest figures (EPA, 1997) among other pollutants. Combining Eqs. (14) and (16) gives the general Eq. (17):

$$\dot{I}_e = \sum_k \sum_j \sum_i x_i \times \left(\frac{\dot{Q}_{i,k}}{\eta_k \times HV}\right) \times \left(\frac{MW_j}{MW_i}\right) \qquad (17)$$

In order to assist process design, it is helpful to have an index independent of process size. This can be achieved by dividing by the total production rate, which gives the Eq. (18):

$$E = \frac{\dot{I}_e}{\sum_n P_n} = \frac{\sum_k \sum_j \sum_i x_i \times \left(\frac{\dot{Q}_{i,k}}{\eta_k \times HV}\right) \times \left(\frac{MW_j}{MW_i}\right)}{\sum_n P_n} \qquad (18)$$
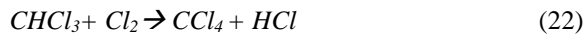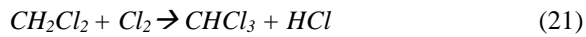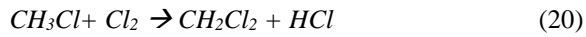
where n = 1,2,3,... represents the product streams in the process.

5. Results

To illustrate the use of the proposed energy index given by Eqs. (16) and (17), it may be helpful for us to consider two case studies. In both cases, the production rates are the almost the same and therefore, the Eq. (18) gives no preference to any alternatives because as stated earlier it is useful for comparing of the processes with different capacities.

5.1. Case Study 1: Chlorination of methane

The production of chloromethane is an important reaction in the petrochemical industry due to their widespread application as solvents. One mole of methane reacts with *four* moles of chlorine to give carbon tetrachloride. The chlorination is a heterogeneous catalytic reaction, taking place in four steps as represented in Eqs. (19) through (22) and the overall Eq. (23):

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl \qquad (19)$$

$$CH_3Cl + Cl_2 \rightarrow CH_2Cl_2 + HCl \qquad (20)$$

$$CH_2Cl_2 + Cl_2 \rightarrow CHCl_3 + HCl \qquad (21)$$

$$CHCl_3 + Cl_2 \rightarrow CCl_4 + HCl \qquad (22)$$

In summary:

$$CH_4 + 4Cl_2 \rightarrow CCl_4 + 4 HCl \qquad (23)$$

The rate constant of chlorination reactions ranges from very low (Eq. 24), such as the chlorination of benzene (Levenspiel, 1999):

$$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl, \ k = 0.412 \qquad (24)$$

to very high, e.g. the chlorination of hydrogen molecules in the presence of light to produce hydrogen chloride. Other chlorination reactions fall within this range.

The chlorination of methane involves a complex network of series and parallel reactions. Reactions (19) to (22) represent a series of reactions with respect to chlorinated species and parallel reactions with respect to Cl_2 (Missen et al., 1999).

A number of factors affecting the kinetics of the chlorination of methane such as the gas flow regime and gas-phase thermal reactions as well as reaction temperature and pressure in industrial applications (Rozanov and Treger, 2010).

The present case study HYSYS process simulator is employed to design a simplified process of the chlorination of methane similar to the technology developed in Germany (Rozanov and Treger, 2010). The thermodynamic and kinetic data have been collected from Goharrokhi et al. (2009). The reactants are well mixed in a CH_4/Cl_2 molar ratio of 0.5 at 25 ºC and 1000 kPa. The chlorination reaction takes place in the gaseous phase at around 430 ºC. In Fig. 1a, the methane and chlorine feeds are heated to 427 ºC before transferring to a plug flow reactor (PFR). The reaction product (marked "To Cooler") is the PFR outlet stream, which is cooled down to 10 ºC before transferring to the separator.

The two-phase flow stream entering the separator is separated into a liquid stream (Product) and the vapor stream (Vapour). The liquid stream is, however, not regarded as finished product and undergoes separate treatment in a downstream plant (not shown).

In an alternative design (Fig. 1b), a heat exchanger is simply added to the process in order to utilize the heat released by the chlorination reactions for heating the feed stream to the PFR reactor and in turn to decrease the temperature of the outlet stream from the PFR (marked "To Cooler"). This allows us to study the environmental effect of this well-known heat recovery system. An alternative to this design involves the recycling of the vapor stream to the beginning of the process (Fig. 1c).

The "Product" flow rates in the original and the alternative designs are 3931 and 3911 kg/h, respectively, about 0.5% difference. The fuel for the boilers is heavy fuel oil (HFO). Based on the composition and characteristics of the HFO, the heat flow attributed to each chemical component in the fuel, $\dot{Q}_i$, was calculated, and data of interest are listed in Table 2. Taking 75% as the conversion efficiency of the boiler (Coulson and Richardson, 2001), it is now possible to calculate the emission rates of all three gases and to compare the three process designs using Eq. (16), with the proviso that $k = 1$ for with and without heat exchanger designs (Figs. 1a, 1b) and k = 2 for heater and compressor (Fig. 1c). In the original design (Fig. 1a), the amount of heat in the heater stream is 4.2×10^6 kJ/h (Table 3). The emission rate of CO_2 to the environment can be calculated using Eq. (16). The results for all three design alternatives can be seen from Eqs. (25) to (29):

$$\dot{I}_j = \frac{3,575,308.8\left(\frac{kJ}{h}\right) \times 0.848\left(\frac{kgC}{kgFuel}\right) \times 44\left(\frac{kgCO_2}{kgmole}\right)}{0.75 \times 42,293\left(\frac{kJ}{kgFuel}\right) \times 12\left(\frac{kgC}{kgmole}\right)} =$$

$$= 350.3 \frac{kgCO_2}{h}$$

$$(25)$$

Table 2. The characteristics of heavy fuel oil and the breakdown of heat value and heat flow
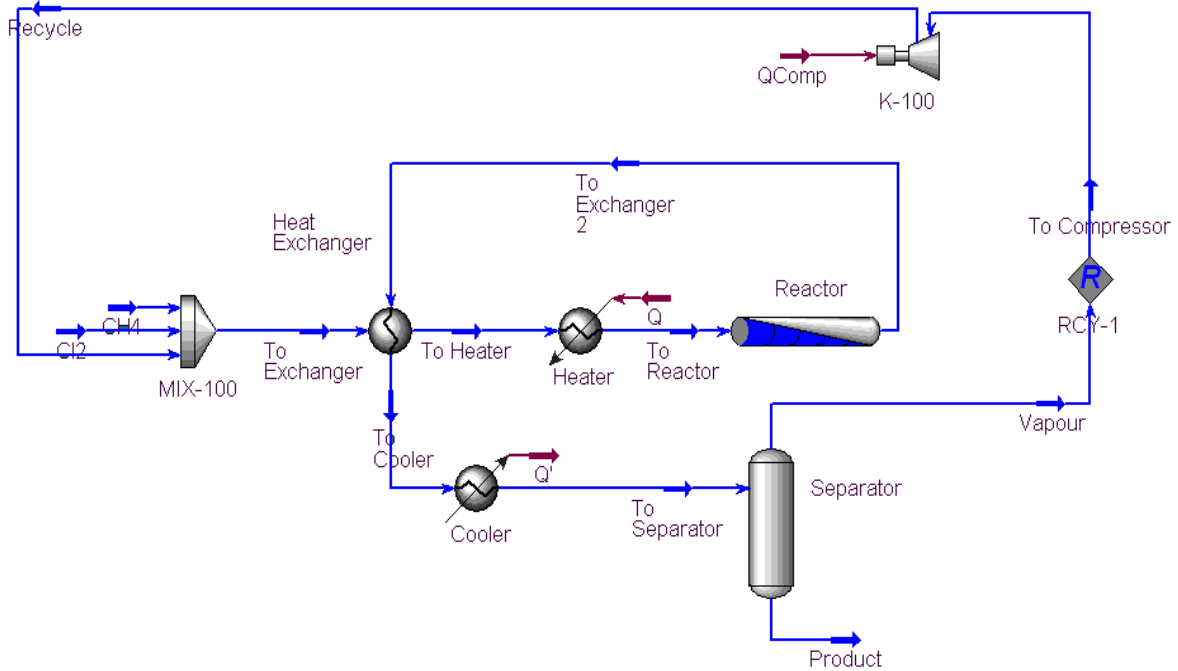
Components	Value	Heat flow, $\dot{Q}_{i,k}$, in kJ/h (without exchanger)	Heat flow, $\dot{Q}_{i,k}$, in kJ/h (with exchanger)	Heat flow, $\dot{Q}_{i,k}$, in kJ/h (with exchanger and recycling)	
				Heat	**Power**
SG	0.941				
HV of fuel	18,200 BTU/lb (**42,293 kJ/h**)				
S	2.7 wt%	113,836.5	3059.1	194,994	107,784
C	84.8 wt%	3,575,308.8	96,078.4	6,124,256	3,385,216
N	0.5 wt%	21,080.8	566.5	36,110	19,960
H	11.93 wt%	502,988.6	13,516.7	861,585	476,245
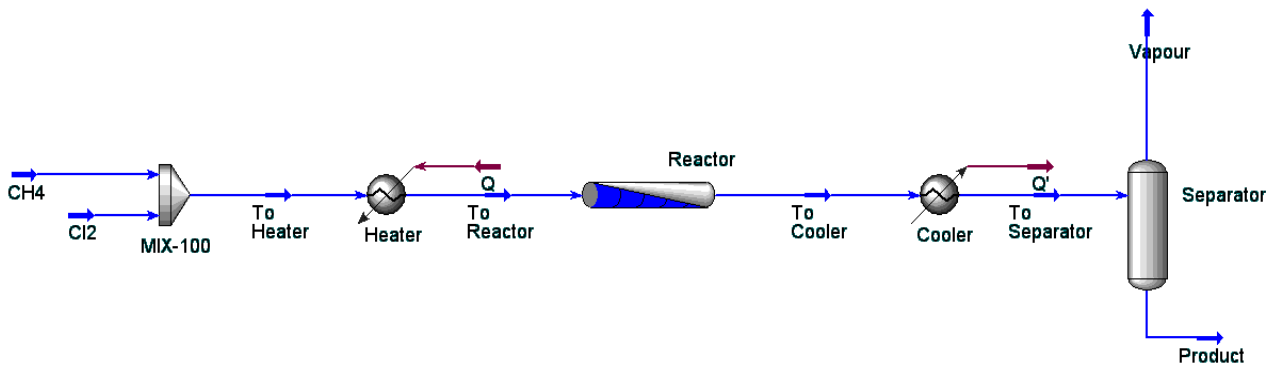
(a)
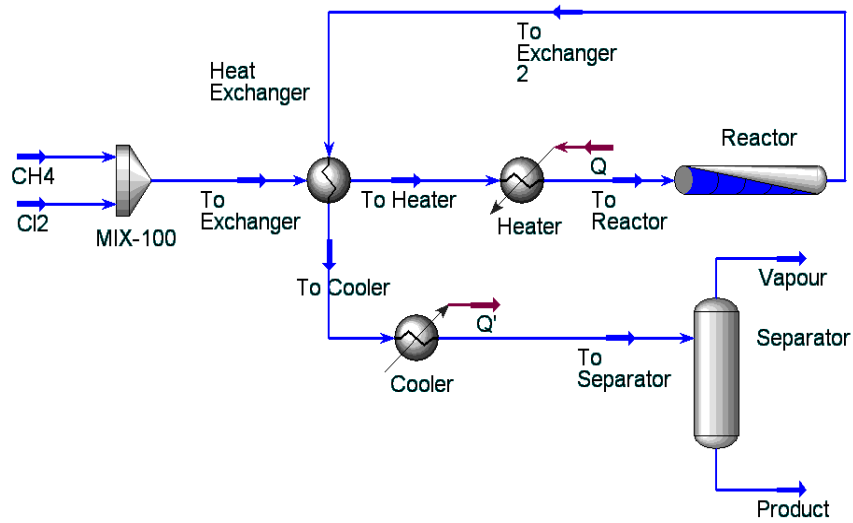
(b)

(c)

Fig. 1. Chlorination of methane: (a) The chlorination design without heat exchanger, (b) Chlorination design with heat exchanger, (c) Chlorination design with heat exchanger and recycling

Similarly, the emission rates for SO_2 and NO_2 are:

$$i_j = \frac{113{,}836.6\left(\frac{kJ}{h}\right) \times 0.027\left(\frac{kgS}{kgFuel}\right) \times 64\left(\frac{kgSO_2}{kgmole}\right)}{0.75 \times 42{,}293\left(\frac{kJ}{kgFuel}\right) \times 32\left(\frac{kgS}{kgmole}\right)} =$$

$$= 0.19\,\frac{kgSO_2}{h}$$

(26)

$$i_j = \frac{21{,}080.8\left(\frac{kJ}{h}\right) \times 0.005\left(\frac{kgN}{kgFuel}\right) \times 46\left(\frac{kgNO_2}{kgmole}\right)}{0.75 \times 42{,}293\left(\frac{kJ}{kgFuel}\right) \times 14\left(\frac{kgN}{kgmole}\right)} =$$

$$= 0.01\,\frac{kgNO_2}{h}$$

(27)

In the design with heat exchanger (Fig. 1b), the quantity of steam heat in the heater is 1.133×10^5 kJ/h (Table 3), and the rate of CO_2 emission to the environment can be estimated using Eq. (16):

$$i_j = \frac{96{,}078.4\left(\frac{kJ}{h}\right) \times 0.848\left(\frac{kgC}{kgFuel}\right) \times 44.01\left(\frac{kgCO_2}{kgmole}\right)}{0.75 \times 42{,}293\left(\frac{kJ}{kgFuel}\right) \times 12.01\left(\frac{kgC}{kgmole}\right)} =$$

$$= 9.4\,\frac{kgCO_2}{h}$$

(28)

Similarly, the emission rates for SO_2 and NO_2 are 5.0 g SO_2/h and 0.3 g NO_2/h, respectively. In the third design (Fig. 1c), we can calculate the gas emissions for both heater and compressor. The total heat flow is 1.121×10^7 kJ/h (Table 3), and the rate of CO_2 emission to the environment can be estimated as:

$$i_j = \frac{6{,}124{,}256\left(\frac{kJ}{h}\right) \times 0.848\left(\frac{kgC}{kgFuel}\right) \times 44.01\left(\frac{kgCO_2}{kgmole}\right)}{0.75 \times 42{,}293\left(\frac{kJ}{kgFuel}\right) \times 12.01\left(\frac{kgC}{kgmole}\right)} +$$

$$+ \frac{3{,}385{,}216\left(\frac{kJ}{h}\right) \times 0.848\left(\frac{kgC}{kgFuel}\right) \times 44.01\left(\frac{kgCO_2}{kgmole}\right)}{(0.75 \times 0.35) \times 42{,}293\left(\frac{kJ}{kgFuel}\right) \times 12.01\left(\frac{kgC}{kgmole}\right)} =$$

$$= 1.547\,\frac{tonsCO_2}{h}$$

(29)

Similarly, the emission rates for SO_2 and NO_2 are 856 g SO_2/h and 49 g NO_2/h, respectively. Table 3 summarizes the results for the above calculated emission rates and heat flows, and also production rates for all three designs. The addition of a heat exchanger results in a significant reduction in the size of both cooler and heater in the alternative designs including a heat exchanger.

Surprisingly, it also reveals that the recycling of vapor to the beginning of the process, as in the alternative design (Fig. 1c), causes a huge increase in energy consumption, particularly by the compressor. As mentioned earlier, due to a lack of information regarding the contribution of fossil fuel types to CO_2 emissions, the EIA conversion factor is based on the average emission for all three types of fossil fuels, and this gives an approximate value. As can be seen in Table 3, the difference between the EIA index and the proposed alternative varies from 25% in the original design to 55% in the alternative containing heat exchanger and recycling process. The reason for this significant variation is that the conversion efficiency of the compressor and boiler are allowed for in the new index.

5.2. Case Study 2: Hydrogenation of unsaturated hydrocarbons

In this case study the hydrogenation of unsaturated hydrocarbon has been modeled by Aspen, HYSYS 2006. The study confirms that Pd is the best catalyst for industrial hydrogenation due to its high conversion factor and its selectivity (Krupka et al., 2006). Pd/α–Al$_2$O$_3$ is also highly selective, without significant deactivation (Seth et al., 2007). The effect of internal diffusion on the rate of hydrogenation of styrene by applying Pd of different particle sizes has revealed that smaller particles are the most effective (Zhou et al., 2007).

Hydrogenation involves a complex catalytic equilibrium which takes place on the heterogeneous surface, and the Langmuir–Hinshelwood rate expression can be used to explain the reaction (Evans and Wennerström, 1994). Ordouei et al. (2014) have used a simplified model to design a hydrogenation plant; Figs. 2a and 2b, and 3a and 3b, illustrate two hydrogenation designs. The kinetic data are summarized in Table 4.

In Fig. 2 the plant feed containing a mixture of hydrocarbons and hydrogen is passed into the first adiabatic PFR reactor. A hydrogen make-up is added to the outlet stream from the reactor to quench the stream and to increase reaction efficiency in the second reactor. The product stream is passed through a shell and tube cooler and then introduced to a flash drum to separate vapor and liquids. The vapor phase is again cooled and further liquid separated in a second flash drum. The liquid from the first and the second flash drums are combined and delivered to a purification section. Most vapor fraction from the second flash drum is compressed and returned to the beginning of the process via a second PFR entrance. The remaining portion of the vapor is mixed with the vapor phase of the flash drum and burned off for heat generation. The light hydrocarbon stream is cooled and separated in a flash drum. The liquid outlet is then sent to a light-end storage tank, while the vapor phase is pressurized and returned to the beginning of the process via the second PFR entrance.

Table 3. Comparison of total energy and total emissions in three designs of the chlorination of methane

	Heat flow to heater (kJ/h)	*Product stream (kg/h)*	*Total emission (kg CO₂/h)*	*Total emission (kg SO₂/h)*	*Total emission (kg NO₂/h)*	*EIA method (kg CO₂/h)*	*EPA method (PEI/h)*
Original design	4.2×10^6	3931	**350.3**	0.19	0.01	**264.6**	**18.06**
Alternative design with heat exchanger	1.1×10^5	3910.4	**9.4**	0.005	0.0003	**6.93**	**0.473**
Alternative design with heat exchanger and recycling	1.1×10^7	3,903.6	**1547**	0.856	0.049	**693**	**47.3**

Table 4. Kinetics data of hydrogenation reactions

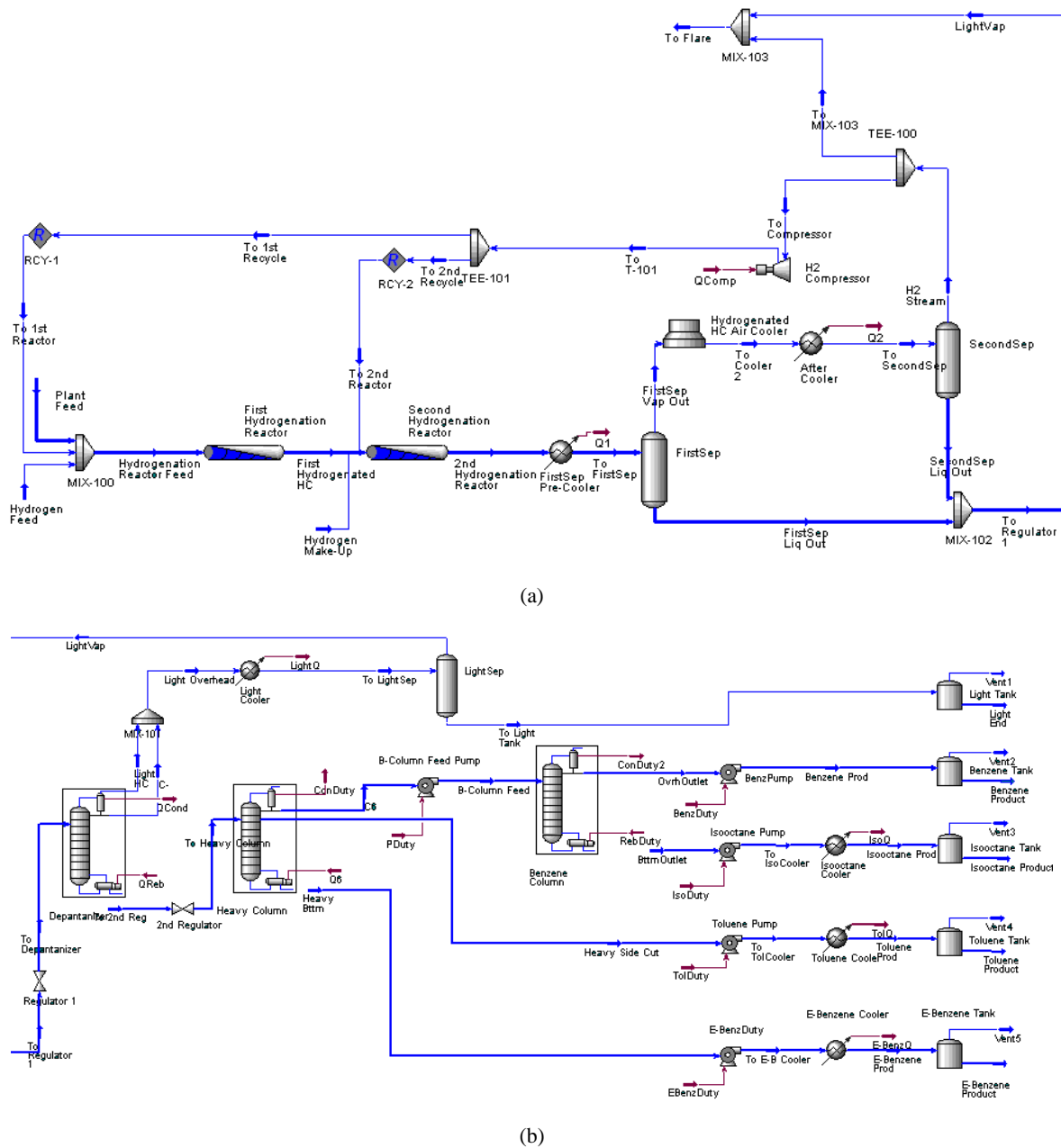| *Unsaturated hydrocarbon*	*k*	*E (J / mol)*	*Reference*
1-Butene	1.482×10^{-5}	34,900	Seth et al., 2007
Isobutene	2.0958×10^{-6}	39,100	Seth et al., 2007
Isooctene	1.23×10^{-4}	10,506	Sarkar et al., 2006
Styrene	0.0415	26,030	Zhou et al., 2007

(a)

(b)

Fig. 2. (a) Hydrogenation process: Original design, reaction and phase separation sections
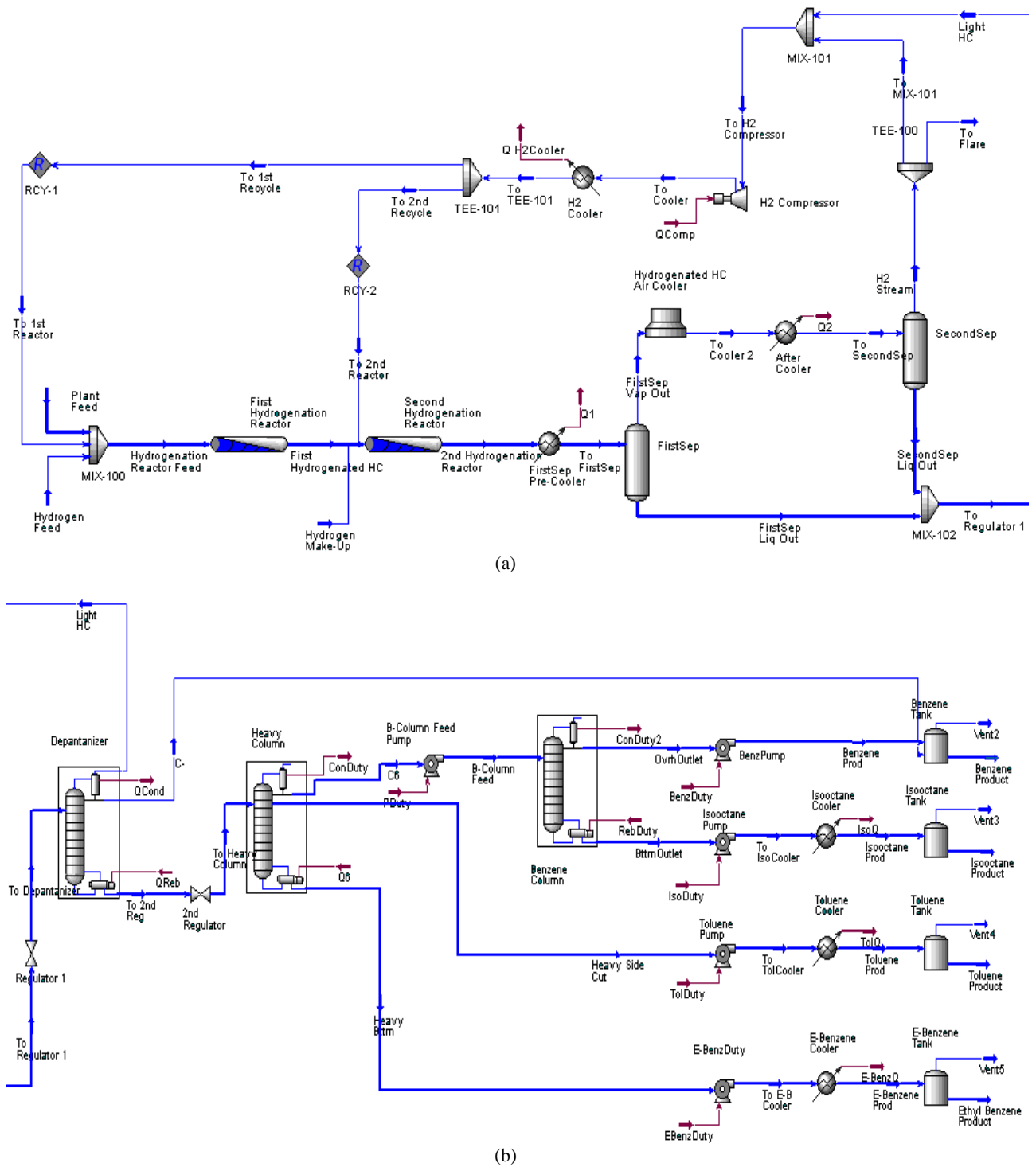(b) Hydrogenation process: original design, purification section

(a)

(b)

Fig. 3. (a) Purification section: Alternative design, reaction and phase separation sections
(b) Purification section: Alternative design, purification section

The heavier hydrocarbon stream is cooled in a shell and tube cooler and introduced to the heavy column, where ethyl benzene and toluene are separated into storage tanks.

The output from the heavy column is separated into benzene and iso-octane and cooled before transferring to storage tanks. In this design, the pyrolysed gasoline is separated into five distinct products, whereas in the alternative design there are four such products. Unlike the original

design, in the alternative design (Figs. 3a and 3b) the overhead and the side-cut from the Depentanizer are compressed and returned to the beginning of the process. Table 5 gives the heavy fuel oil characteristics and heat flows for each design. The energy impact has been calculated for both processes, and the results are summarized in Table 6. The energy impact on the environment arising from heat and power consumption are each lower in the original than in the alternative design.

6. Discussions

This paper presents a screening index for the quantification and selection of an optimal process in terms of energy consumption and economic design, leading to the conservation of fossil fuel resources and preservation of clean air. The index has been applied to two different case studies.

The first offers three alternative process designs of which the second, with heat exchanger and without a recycling process, emits fewest polluting gases to the atmosphere by a factor of about 40, compared to the original design without heat exchanger and recycling process. In the case of the alternative design with both heat exchanger and recycling process the factor becomes 165. This means the design with heat exchanger and without recycling process is not only the most economic, but also it helps to preserve fossil fuel resources and clean air– the basic concept of sustainability.

The energy impact of the design alternatives has been assessed using the new proposed index and also by the EIA and EPA methods. All three methods indicate that the energy impact of the alternative hydrogenation design is profound. In addition, the newly proposed index offers greater detail about the various emissions of the processes and gives a more accurate assessment. Unlike the EIA and EPA methodologies, there is no linear relationship between energy consumption and gas emission, as is seen from Table 3. For instance, in the chlorination design the energy consumption between Figs. 1c and 1b differs by a factor of 100. The corresponding emission ratio is however 165.

The second case study considers an alternative design for the hydrogenation of unsaturated hydrocarbons. In the original design the overhead of the heavy column is sent to a benzene column, whereas in the alternative design the overhead and the side-cut of the Depentanizer are recycled back to the start of the process. The energy impact of both alternatives has been assessed using the new proposed index and the EIA and EPA methods. All three methods agree that the energy impact of the second alternative is the greater. In addition, the new proposed index offers further details about the emissions of the processes and gives a more accurate assessment. The new methodology has a number of other advantages:

(a) it is a simple and user-friendly tool for the quantification and measurement of emission rates;

(b) it is accurate and calculates precisely the emission rates of CO_2, SO_2 and NO_2;

(c) it requires relatively readily available data, such as fossil fuel composition and heat value, heat flow through a heat exchanger, or electric power consumption of the electromotors of pump compressors, fans, blowers etc.;

(d) it is applicable to both the early stages of process design where there is a lack of process data, as well as to the estimation of emission rates in operating plant due to energy consumption by process equipment such as pumps, compressors etc.;

(e) it is not limited to chemical processes and can be extended to the generation of heat or electricity from fossil fuels;

(f) there is no need to measure fuel flow rate;

(g) it provides detailed information in terms of the environmentally friendliness of processes;

(h) unlike the EPA and EIA methods, the new index provides no linear relationship between energy consumption and gas emissions;

(i) the new index demonstrates that an economic design can be linked to sustainability.

7. Conclusions

The new proposed energy index ranks process alternatives in terms of sustainable energy and environmental impact. It provides an effective tool for decision makers to identify the most sustainable process design.

The index can be used for both existing processes and to identify potential new designs, and it presents a vital tool for minimizing adverse environmental effects in order to combat climate change and maintain good air quality. The index is also useful for energy efficiency in terms of improving energy intensity and environmental effects.

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Table 5. The characteristics of heavy fuel oil and the breakdown of HV and heat flow

Components	Value	Heat flow, $\dot{Q}_{i,k}$, in kJ/h (original design)		Heat flow, $\dot{Q}_{i,k}$, in kJ/h (alternative design)	
		Heat	Power	Heat	Power
SG	0.941				
HV of Fuel	18,200 BTU/lb (**42,293 kJ/h**)				
S	2.7 wt%	848,693	4,207	889,500	27,898
C	84.8 wt%	26,655,234	132,125	27,936,877	876,193
N	0.5 wt%	157,165	779	164,722	5,166
H	11.93 wt%	3,749,964	18,588	3,930,271	123,266

Table 6. Comparison of emission impacts in both designs of hydrogenation process

	Total energy consumption (kJ/h)	Product stream (kg/h)	Total emissions (kg CO_2/h)	Total emissions (kg SO_2/h)	Total emissions (kg NO_2/h)	EIA method (kg CO_2/h)	EPA method (PEI/h)
Original design	31.59×10^6	12,427	**2,650**	1.46	0.08	**1,990**	135,819
Alternative design	33.98×10^6	12,482	**2,984**	1.65	0.09	**2,141**	146,090

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