# Measurement of the Sustainability Performance of Chemical Manufacturing Processes

# Measurement of the Sustainability Performance of Chemical Manufacturing Processes:

*Best Practice*

By

Mohammad Hossein Ordouei

Cambridge Scholars Publishing

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—Mohammad Hossein Ordouei

# PREFACE

As I embark on writing this book, the global consciousness surrounding climate change is reaching new heights. Governments worldwide are implementing corrective measures to address impending disasters. The commencement of this book coincided with COP26, which served as a beacon of hope amid the challenges posed by global warming.

COP, short for 'Conference of the Parties,' is an International Relations term referring to a committee established after signing an international treaty. This committee is entrusted with decision-making regarding the implementation of the treaty. At COP, politicians, diplomats, and national representatives are crucial attendees, but various other groups also participate to influence outcomes. Fossil fuel lobbyists often aim to safeguard their industry, while environmental defenders and Indigenous groups advocate for territorial protection. Climate organizations, like Global Witness, push for ambitious climate action. Despite this diverse participation, barriers such as economic, legal, and physical challenges can limit the involvement of environmental activists and civil society organizations. Every COP is identified by its numerical order in the series, such as COP26 for the 26$^{th}$ meeting. Any fresh agreements resulting from COP typically bear the name of the host city, like the 2021 Glasgow Climate Pact (Global Witness, 2023).

The 20 strongest countries joined in November 2021 at the COP26 summit. The Glasgow Climate Pact, adopted by nations, seeks to usher in a decade of climate action and support. It encompasses measures to enhance resilience, curb emissions, and provide financial support. Nations reaffirmed the $100 billion annual pledge and committed to bridging the gap between existing emission reduction plans and the necessary measures to limit the global temperature rise to 1.5 $^{o}$C. Notably, the pact calls for the phasedown of unabated coal power and inefficient fossil fuel subsidies, marking a crucial milestone (UNFCCC, 2021).

The global average temperature in 2022 was approximately 1.15 $^{o}$C higher than **preindustrial** levels (Chu, 2023), placing industries at the forefront of

the warming crisis. This compels scientists and engineers to urgently seek effective solutions to resolve the global warming challenge.

The present book delves into these issues, along with emphasizing risk reduction and pollution prevention. This book provides several case studies merely for the sake of simplicity for better understanding the methodologies presented in the book and their applications.

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# INTRODUCTION

The growing awareness of industrial and environmental hazards has spurred a global movement by governments to combat climate change, acid rain, ozone depletion, and harmful gas emissions. These concerns weigh heavily on environmentalists, scientists, engineers, decision-makers, governments, and the public alike. The goal is to enhance the health of both humans and animals, safeguard the environment and natural resources for future generations, economize resources, and, above all, adhere to and respect established laws and policies.

Recent years have witnessed an extensive array of global environmental catastrophes. Research indicates that the twenty most expensive extreme weather incidents in 2023, from Hawaii's wildfires to Malawi's cyclone, accrued over $200 billion in damages. Tragically, countries most affected were those with minimal contributions to the climate crisis or limited coping and rebuilding capacities (Dodds, 2023; Horton, 2023; Hughes, 2023).

The unprecedented heatwaves, floods, droughts, storms, and wildfires were linked to human-induced global warming. In 2023, among various nations, **the UK, Germany, and China** experienced their warmest year on record (Wu, 2023; Gerretsen, 2023).

In Canada, the government's initial national disaster risk assessment in May 2023 highlighted the risks from earthquakes, wildfires, floods, and the ripple effects of pandemics like COVID-19. Though not specifying figures for 2023's toll, the report stressed the mounting frequency and severity of natural disasters, posing growing concerns for Canada and the world (Government of Canada, 2023). Additionally, a CBC News report estimated that floods, droughts, and storms might cost Canada's economy $139 billion over the next three decades, with manufacturing and distribution being most affected by water-related climate disasters (The Canadian Press, 2022).

In the U.S., the National Oceanic and Atmospheric Administration (NOAA) reported a record-setting 15 billion-dollar climate disasters in 2023, totaling over $57.6 billion in damages. These events, ranging from extreme rainfall to wildfires, resulted in at least 114 deaths, excluding the Maui fire that claimed more than 100 lives (Statista, 2023).

The Institute of Economics & Peace's Ecological Threat Report identified 27 countries with low societal resilience and high ecological threats, eight of which faced catastrophic conditions: **Burundi, Central African Republic, Chad, Republic of the Congo, Somalia, South Sudan, Uganda, and Yemen**. These nations, home to around 146 million people, endured severe droughts, floods, famines, conflicts, and displacements due to the climate crisis. They have minimal capacity to cope or rebuild and contribute the least to global greenhouse gas emissions, necessitating urgent international support (Thomson, 2023; Horton, 2023).

Similarly, the occurrences of industrial accidents due to the lack of safe working habits have been noteworthy. The Coalition to Prevent Chemical Disasters reported over 30 chemical accidents in the U.S. in the initial seven weeks of 2023, almost one every day and a half (Gillam, 2023).

In 2022, fire-related incidents in the U.S. led to 3,790 civilian deaths, 13,250 injuries, and 96 on-duty firefighter fatalities. This marked the highest firefighter death toll since 2013 (NSC Injury Facts, 2023). Meanwhile, the private sector reported 2.6 million non-fatal workplace injuries in 2021, with the healthcare industry accounting for the highest number (453,200). The rate of workplace injuries remained constant at 2.7 per 100 full-time equivalent workers from 2020 (Work Injury Source, 2023).

Today, global warming is the foremost challenge in human history, as 2023 saw a global average temperature of 1.2°C above the pre-industrial level, setting a record (Gerretsen, 2023). These occurrences underscore the urgency of curbing greenhouse gas emissions and bolstering resilience to climate impacts (Wu, 2023; Gerretsen, 2023).

The term "**pre-industrial**" places industries at the forefront of the warming crisis. A rise of 1.2 ºC above the **pre-industrial** era signals the substantial responsibility that scientists and engineers shoulder to find solutions. Evidently, there isn't a single immediate fix, so collective efforts are essential.

The statistical data and conclusions have spurred the author's action. As an experienced chemical engineer in the design and operation of chemical, petroleum, and mining processing industries and a skilled teacher in the field, I have authored this book for seasoned process systems engineers (PSEs) aiming to contribute to this imperative cause.

The book presents a framework for quantifying the sustainability performance of chemical processes, consisting of hybrid methodologies called Composite

Sustainability Indicator (CSI), focusing on environmental protection, risk reduction, and emissions cutback.

Sustainability is defined as 'meeting the needs of the present without compromising the ability of future generations to meet their own needs.'

The CSI employs the Waste Reduction (WAR) Algorithm to evaluate the potential environmental impacts or PEI, risk assessment, and energy intensity models.

The author's contribution includes:

- Introducing the risk assessment model, which enables the PSEs to design inherently safer processes (ISD).
- The energy intensity index, derived from mass and energy balance calculations.
- Integrating the models above and the WAR algorithm into the conceptual process design where the detailed operating data are unavailable.
- Aggregating these methodologies into a value called Key Process Indicator, KPI.

The KPI is a technical concept representing a process' sustainability performance, making it possible to perform a KPI-Profitability analysis and rank the process design alternatives based on their sustainability performance. Multiple case studies prove the effectiveness of individual and composite methodologies.

The book is organized in the following chapters:

- Chapter 1: Computer-Aided Modeling and Simulation Process Design. This chapter familiarizes the respected readers with the process flowsheets and using computer simulator software packages to design them, such as Aspen HYSYS, Aspen Plus, ChemCAD, etc.
- Chapter 2: Interpretation of Langmuir-Hinshelwood Mechanism. This book does not provide chemical engineering core courses. However, due to the broad applications of heterogeneous equilibrium catalytic reactions in chemical and upgrading processes, the author provides a deep understanding of the *Langmuir* adsorption isotherm, surface phenomena, and nano catalysts' characteristics and proposes a strategy to streamline such a complex mechanism. A case study

illustrates the simplified hydrogenation heterogeneous catalytic reaction.

- Chapter 3: Pollution Prevention and Environmental Protection: A literature review that provides historical background and the importance of resource preservation, pollution prevention, and environmental protection.
- Chapter 4: Potential Environmental Impacts and Waste Reduction (WAR) Algorithm: The WAR algorithm is an existing approach to minimize waste reduction at the primitive design stage of a chemical process. The WAR algorithm employs the concept of the Potential Environmental Impacts of product and waste streams to determine the environmental consciousness of a chemical process.
- Chapter 5: Global Warming: Energy Index: The author first presented and published this energy index, which originates from mass and energy balance calculations, marking a departure from the conventional chemical process design paradigm to focus more on a thermal dilemma perspective.
- Chapter 6: A Risk Assessment and Hazard Reduction Methodology at the Conceptual Design Stage of a Chemical Process: The author first introduced and published this mathematical risk assessment model, a robust screening tool for designing and retrofitting inherently safer processes.
- Chapter 7: Profitability Analysis: Designing profitable chemical processes to attract investors is imperative. This chapter provides a general understanding of the process economy and profitability.
- Chapter 8: Introduction to Composite Sustainability Indicator (CSI): This chapter provides a clear understanding of the CSI and its three pillars, i.e., environment, risk, and energy indices. The introduction is followed by case studies to illustrate the methodology when there is no conflict between the pillars.
- Chapter 9: Composite Sustainability Indicator (CSI)-Complex Case Studies: As the units of three tenets (WAR algorithm, Risk, and Energy Indices) are different, combining them seems impossible, especially when there are conflicts between them. This chapter explains how to use the Analytical Hierarchy Process (AHP) and successfully applies it to complex refinery processes.
- Chapter 10: Artificial Intelligence (AI) and CSI:

The author has extensively employed the Aspen Plus and Aspen HYSYS advanced process simulators (Aspen Technology Inc., 2023) for the case studies in this book. As such, he used the WAR GUI (2008) to estimate the

potential environmental impacts (Chapter 4) of material streams of chemical processes.

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# CHAPTER 1

# COMPUTER-AIDED MODELING AND SIMULATION IN PROCESS DESIGN

This chapter provides general knowledge of computer-aided modeling, simulation, and design in chemical engineering. It by no means gives information on the design of a chemical process; for that, the software development companies arrange several training workshops that enable the participants to do so perfectly.

In this chapter, the respected readers will learn about the steps of the chemical process design and requirements, including raw material quality and quantity, the compositions and conditions of the inlet streams, and the process plant's boundaries.

## 1.1 The advantages of computer simulators

A Process Systems Engineer (PSE) is an expert in most areas of the chemical engineering field, including modeling and simulating a chemical process using computer-aided design software. The objectives of a PSE vary from design to the optimization and control of a process. The PSE has a deep understanding of mathematical modeling, data analytics, heat and material balance, reaction thermodynamics and kinetics, heat and mass transfer, equipment sizing, hydraulic calculations, flowsheet design, design and development of PFD (Process Flow Diagram), and P&ID (Piping and Instrumentation Diagram); cost estimation; profitability analysis.

The design of a chemical process starts from a design basis, such as chemical compositions and conditions of raw material and product streams, raw material and product quantity, and quality. The product characteristics are determined by learning about customer demands and market research. The location of a chemical process plant may be anywhere, regardless of tropical or cryogenic climates. One may find several chemical reactions to produce a single product; however, choosing the best reaction relies on several factors, such as the availability of raw materials, catalysts, product

quality, and market price. The selection of raw materials depends on price, quality, and availability.

The PSE can design process flowsheets by gathering the minimum required data, such as compositions and conditions of material streams, chemical reactions, the energy needed for the reactions, reaction thermodynamics & kinetics, and catalysis. The flowsheet represents a multi-stage process, materials streams, phase separation, and purification. The stream conditions include pressure, temperature, and flow rate. For instance, the condition of a feed stream to an oil refining plant is given below:

**Pressure:** **30 kg/cm$^2$**
**Temperature”** **100 ºC**
**Mass Flow Rate:** **12,500 kg/h**

Attention should be paid to the units. The above values are based on the International System of Units (SI), sometimes called Metric Units. Imperial Units is another measurement system still being used in the USA and Canada. So, the units must be consistent with the system of measurements, and conversion factors must be used if necessary.

Fig. 1.1 shows the flowsheet of an upgrading process and provides general information on the material stream routes, reactor type, other equipment blocks, and labels.

The flowsheet is saved as a .DXF file and then converted to a PFD using the AutoCAD software. The .DXF file must be opened in an AutoCAD environment to apply required changes and saved in AutoCAD as a Process Flow Diagram.

Table 1.1 provides a typical composition of raw materials (feed) stream to a process plant’s Battery Limit (BL). The BL of a plant within a chemical manufacturing complex is an imaginary boundary where the material and energy streams enter and/or exit.

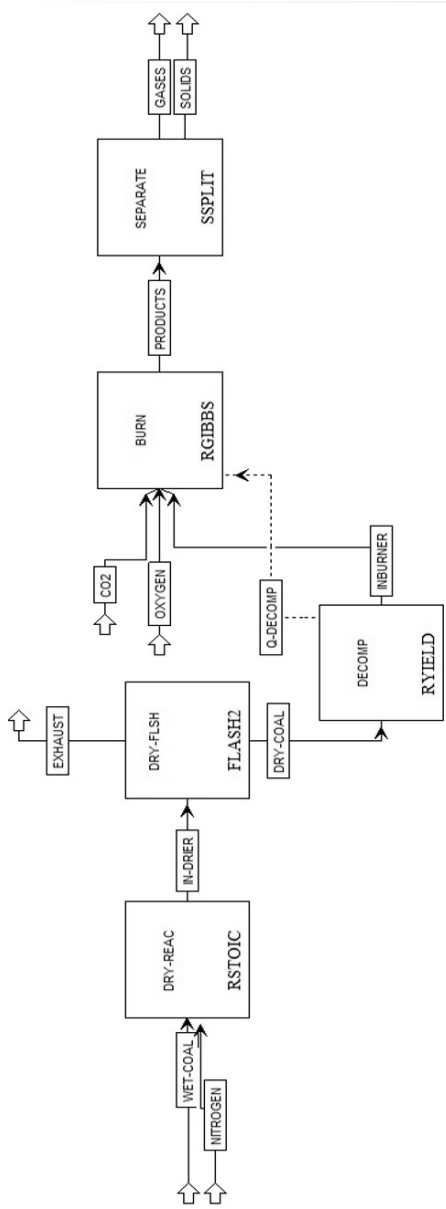



**Fig. 1.1** The Process Flow Diagram (PFD) of a Coal Gasification By Aspen Plus. This process is not necessarily the best design.

**Table 1.1** The chemical composition of a hydrocarbon feed stream to an upgrading process (Ordouei, 2014)

| Components | Hydrocarbon Feed Stream (wt %) |
|---|---|
| Iso-Butane | 1.02 |
| n-Butane | 0.79 |
| Iso-Pentane | 0.96 |
| n-Pentane | 0.17 |
| Iso-Butene | 0.91 |
| Iso-octene | 10.92 |
| 1-Butene | 0.54 |
| Styrene | 15.53 |
| Ethyl-Benzene | 2.31 |
| Benzene | 48.01 |
| Toluene | 18.84 |

Each step of the PFD requires complex mathematical equations to be solved. The mathematical formulation of a phenomenon, such as fluid flow in a pipe, is called modeling, and solving the equation (the mathematical formula) is called simulation.

Therefore, designing industrial chemical processes requires solving tens of thousands of mathematical equations simultaneously. This list of activities requires several process engineers to fulfill all tasks, which is time-consuming and cost-effective, yet it is almost impossible to solve such enormous equations by hand calculation.

The good news is that high-speed computers are available today at reasonable prices. However, hi-tech computers can solve only one part of the issue; another equally important factor is needing for innovative software packages that enable process engineers to design chemical manufacturing processes with high precision and accuracy.

Researchers have developed many mathematical solvers, such as POLYMATH, for quick calculations of algebraic equations, linear and non-linear systems analysis, and ordinary differential equations (ODE) with appreciable accuracies. MATLAB is a widely used software with the capabilities mentioned above, as well as partial differential equations (PDE) and optimization.

There are several helpful solvers of this kind; however, process engineers demand more advanced packages to design multi-million dollar chemical plants. The following section introduces some brilliant Process Simulation Software Packages that chemical process designers extensively use to fulfill this crucial task.

## 1.2 Process simulators

A number of Process Simulation Software Packages are commercially available and mature enough to solve all mathematical models and sets of ODE, PDE, and more simultaneously with high degrees of confidence in just minutes using complex algorithms. Examples include Aspen Plus and HYSYS (Aspen Technology Inc., 2023), ChemCAD (Chemstations Inc., 2023), CADSIM Plus (Aurel Systems Inc., 2019), and Pro II (AVEVA Group, 2023), which are widely used in chemical, petroleum, biomass process, petrochemical, gas processing industries, and power plants. These software packages provide fashionable graphical simulation possibilities for chemical process engineers; their difference is just a matter of taste. There are various process simulators that industrial designers use for similar purposes; these simulators include mining processing, pulp and paper, water treatment, and wastewater treatment, which are out of the scope of this book.

Therefore, chemical process designing companies, known as process licensors, prefer to furnish their corporations with hi-tech computers and technologies and such process simulators to maximize process design efficiency and corporate profitability. The advanced process simulators mentioned above provide the end users with a library and reliable data bank, which enable process systems engineers to design complex process flowsheets, including:

A. Physical properties data and models
B. Chemical properties data
C. Thermodynamic properties data
D. Transportation properties information
E. Default various equipment with proprietary calculations for sizing purposes
F. Precise capital and revolving cost estimations

ASPEN HYSYS, along with other process simulators, facilitates process modeling, simulation, design, optimization, and equipment sizing of chemical and refinery plants. These simulators are extensively used in many

chemical manufacturing plants and are among the essential qualifications many big companies consider for the new candidates they wish to hire.

A typical process simulator software provides chemical engineers with exceptional information and capabilities, such as:

**A. Physical and Transport Properties:** These properties include Component Name, Family Class, Chemical Formula, CAS Number, UNIFAC Structure, Base Properties (Molecular Weight, Normal Boiling Point, and Density), Critical Properties (Temperature, Pressure, Specific Volume, and Acentricity), liquid and vapour densities, viscosity, surface tension, and thermal conductivity.

Fig. 1.2 shows the information on the physical properties of i-Butane provided by Aspen HYSYS. The software user can edit the properties of a substance using the "Edit Properties" button highlighted in Fig. 1.2. Editing a chemical's properties is helpful if the chemical does not exist in the software library. Then, it may be considered a hypothetical element.

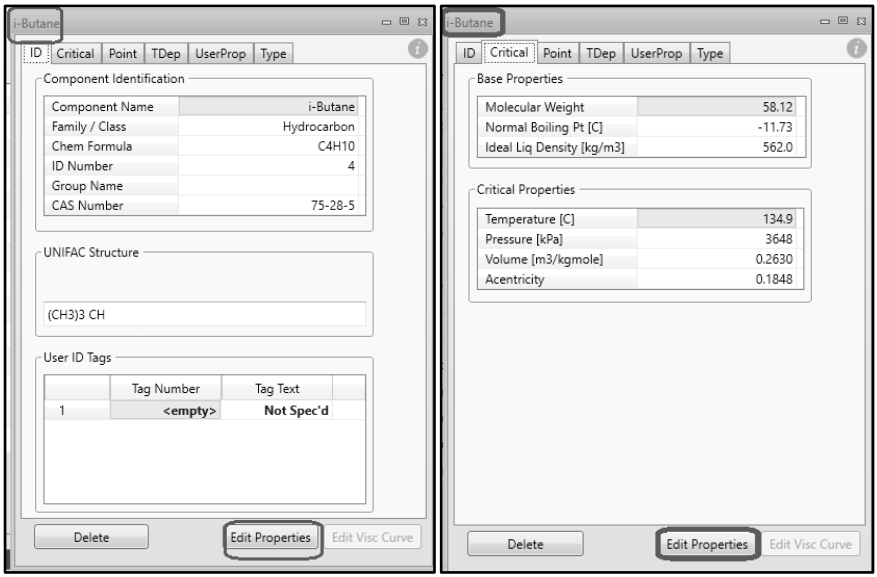



**Fig. 1.2** Physical properties of Iso-Butane from Properties of the Aspen HYSYS.

**B. Thermodynamic Properties Information:** These properties are essential to predict the behavior of a chemical component. These properties include but are not limited to Vapour Enthalpy, Vapour Pressure, Gibbs Free Energy, Heat of Formation, and Heat of Combustion.

Fig. 1.3 shows the information on the thermodynamic properties of i-Butane provided by Aspen HYSYS.

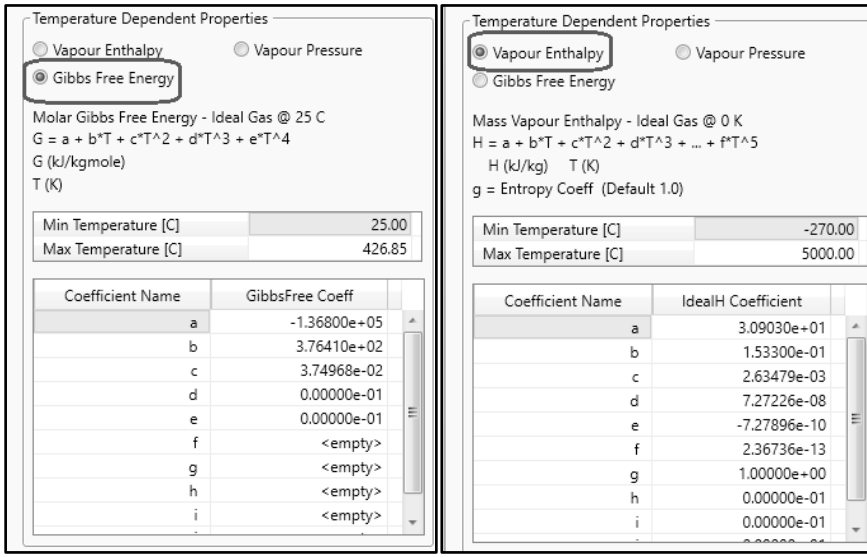



**Fig. 1.3** Thermodynamic properties of Iso-Butane from Properties of the Aspen HYSYS.

**C. Fluid Packages:** A fluid package is combined from a list of chemicals in a stream (Components Lists) and several tasks associated with a specific process (Property Package). A fluid package includes data related to pure component flash and physical property calculations and is assigned to a flowsheet used in a simulation. Fig. 1.4 represents the fluid package within the Aspen HYSYS Process Simulator.

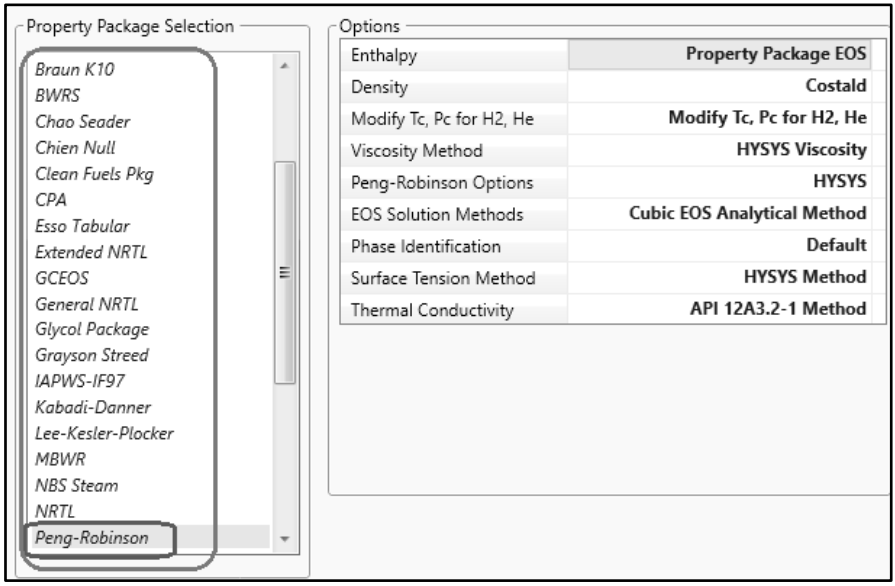
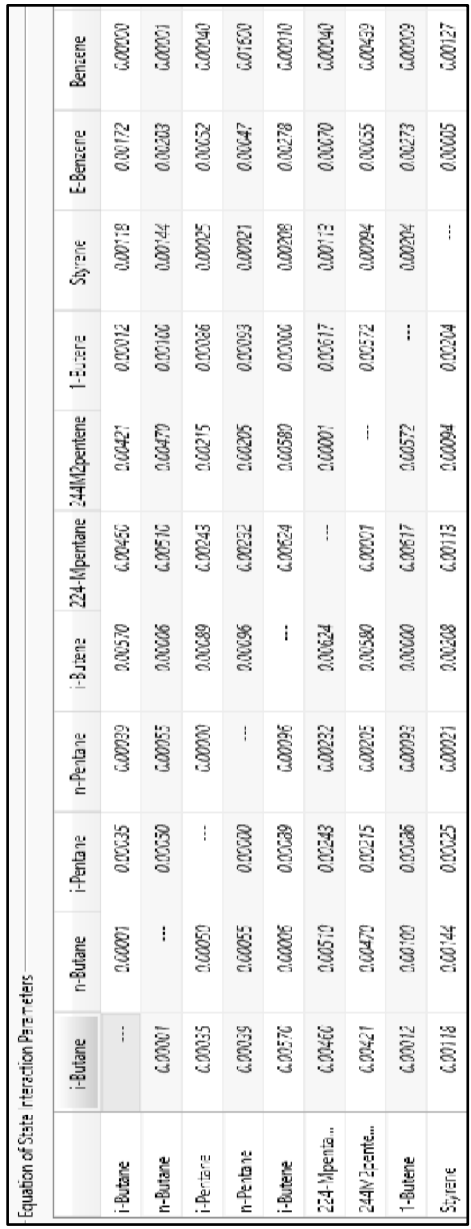



**Fig. 1.4** Fluid Package for a hydrocarbon mixture; Aspen HYSYS.

On the "Property Package Selection," there are various property packages for the existing component list based on the type of the components, e.g., electrolyte solution.

On the "Option" side of the pan, various calculation methods exist for estimating enthalpy, density, viscosity, etc. An expert process engineer must be highly knowledgeable in thermodynamics to make the right decision regarding Fluid Package Selection. For example, the Peng-Robinson property package gives precise results when a hydrocarbon mixture is concerned.

In addition, when there is more than one chemical component in a process stream, it is more likely to observe interactions between the components. This kind of interaction is common in almost all chemical process industries. Therefore, the simulator calculates the Binary Coefficient based on the selected Fluid Package and the Equation of State Interaction Parameters (Fig. 1.5). It is possible to employ multiple fluid packages in one simulation by assigning a property package to a component list.



Equation of State Interaction Parameters

| | i-Butane | n-Butane | i-Pentane | n-Pentane | i-Butene | 224-MPentane | 244MPentene | 1-Butene | Styrene | E-Benzene | Benzene |
|---|---|---|---|---|---|---|---|---|---|---|---|
| i-Butane | --- | 0.00001 | 0.00035 | 0.00039 | 0.00570 | 0.00450 | 0.00421 | 0.00012 | 0.00118 | 0.00172 | 0.00020 |
| n-Butane | 0.00001 | --- | 0.00030 | 0.00055 | 0.00006 | 0.00510 | 0.00470 | 0.00100 | 0.00144 | 0.00203 | 0.00001 |
| i-Pentane | 0.00035 | 0.00050 | --- | 0.00000 | 0.00089 | 0.00243 | 0.00215 | 0.00086 | 0.00025 | 0.00052 | 0.00040 |
| n-Pentane | 0.00039 | 0.00055 | 0.00000 | --- | 0.00096 | 0.00252 | 0.00205 | 0.00093 | 0.00021 | 0.00047 | 0.01500 |
| i-Butene | 0.00570 | 0.00006 | 0.00089 | 0.00096 | --- | 0.00624 | 0.00580 | 0.00006 | 0.00208 | 0.00278 | 0.00010 |
| 224-Mpentane | 0.00460 | 0.00510 | 0.00243 | 0.00252 | 0.00624 | --- | 0.00001 | 0.00617 | 0.00713 | 0.00070 | 0.00040 |
| 244MPentene | 0.00421 | 0.00470 | 0.00215 | 0.00205 | 0.00580 | 0.00017 | --- | 0.00572 | 0.00984 | 0.00055 | 0.00439 |
| 1-Butene | 0.00012 | 0.00100 | 0.00086 | 0.00093 | 0.00000 | 0.00617 | 0.00572 | --- | 0.00204 | 0.00273 | 0.00009 |
| Styrene | 0.00118 | 0.00144 | 0.00025 | 0.00021 | 0.00208 | 0.00713 | 0.00984 | 0.00204 | --- | 0.00005 | 0.00127 |

**Fig. 1.5** Binary Coefficient of a hydrocarbon mixture; Aspen HYSYS.

**D. Reaction Modeling and Reactor Design:** Fig. 1.6 shows "Reaction Set" dialogue box with a Solver Method and Active Reactions selected. It is possible to model multiple reactions in one reactor. Fig. 1.6 shows that Aspen HYSYS modeled four catalytic reactions.

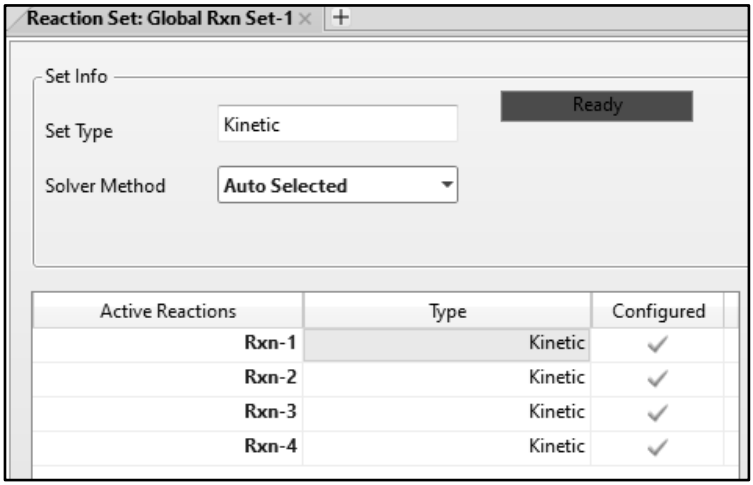



**Fig. 1.6** Reaction Set containing four kinetic reactions, modeled by Aspen HYSYS.

The process simulator enables chemical engineers to model complex chemical reactions by providing the required information for the software. These crucial data include reaction equation, reaction stoichiometry, thermodynamics of the reaction, kinetic data of the forward and reverse reactions, reaction phase, temperature and reaction of the activation energy, catalysis data, including porosity, particle diameter, particle sphericity, solid density, solid heat capacity, void fraction, reactor volume and so on.

A chemical reaction's required kinetic and thermodynamic data can be entered into the simulator by clicking on the Active Reaction and filling each box (Fig. 1.7).

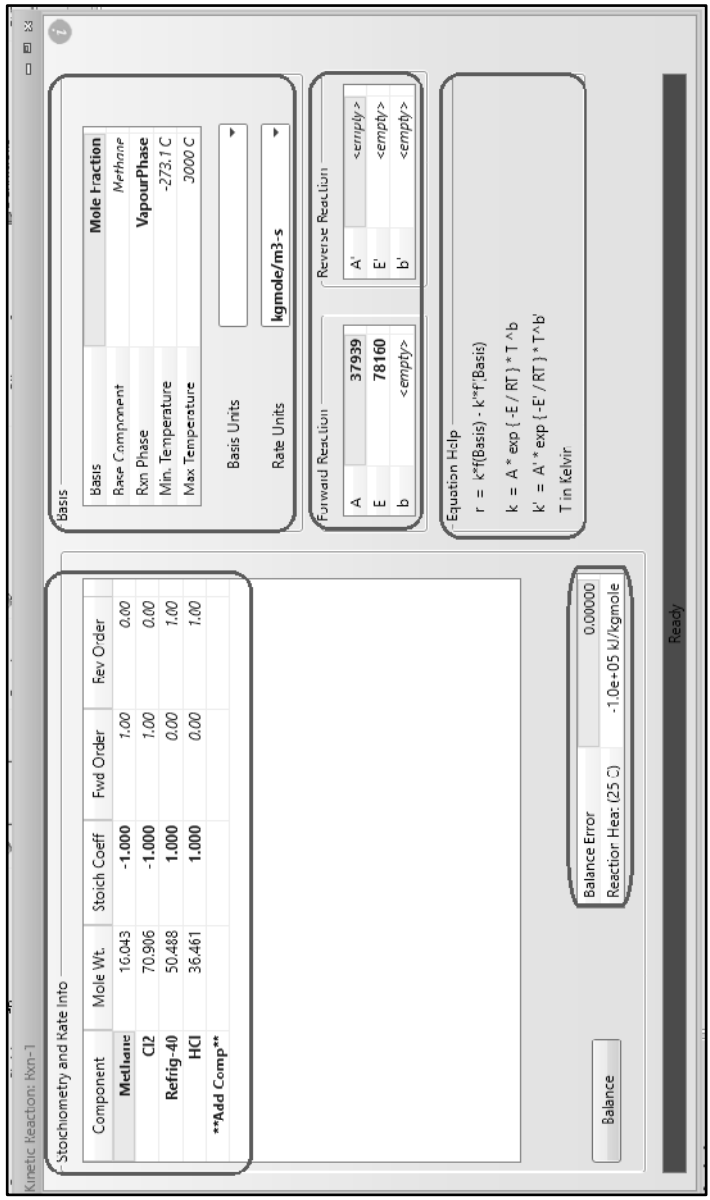



**Fig. 1.7** Dialogue box of kinetic data for heterogeneous catalytic equilibrium reaction, by Aspen HYSYS

Examples include the stoichiometry Coefficient of methane chlorination reaction, Base Component (here methane), Reactants, Products, Reaction Phase, Temperature Range, Activation Energy, and Frequency Factor of Forward and Reverse reactions.

The catalyst's characteristics, such as porosity, diameter, density, and sphericity, must be entered in the Cataltsy Data dialogue box (Fig. 1.8).

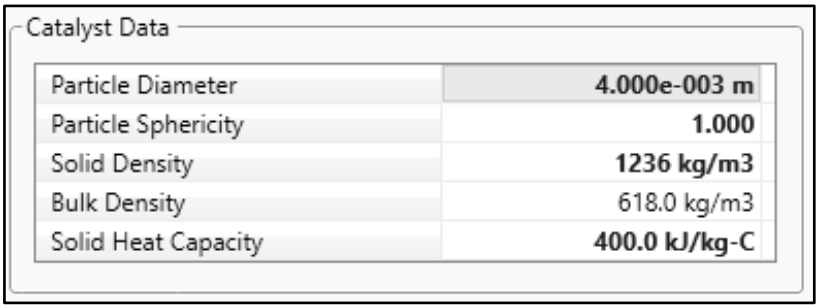



**Fig. 1.8** Catalyst Data dialogue box; Aspen HYSYS.

**E. Equipment Sizing:** Equipment modeling, design, and sizing have significant potential for a process simulator, such as Aspen HYSYS. Fig. 1.9 shows some required data for designing and sizing a plug flow reactor (PFR). The values of Tube Dimensions, Pressure Drop, Tube Packing, and Duty Parameters are required to size a PFR. Since the reactor is exothermic, its duty is zero, so no heat is applied.

The respected readers should bear in mind that the reactor size calculated by a process simulator only gives a good approximation of the tube packing volume. The manufacturing companies develop essential documents that provide their design engineers with precise, detailed design calculations based on the lessons learned from their previous designs. The reactor volumes designed and sized by these manufacturers differ from the calculated volume in practical cases. The extra volume is due to the consideration of design margins for maintenance spaces, reactor heads at both ends and inlet and outlet lines.

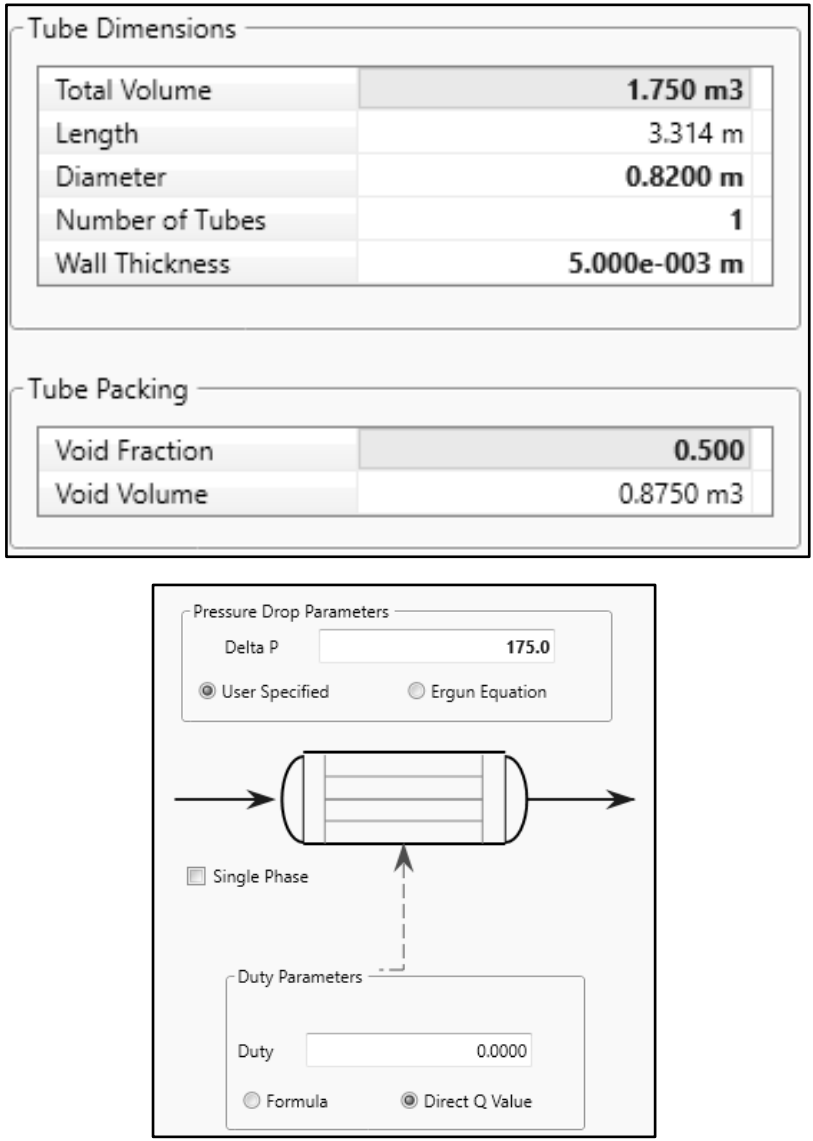



**Fig. 1.9** Quick reactor sizing; Aspen HYSYS.

**F. Process Flowsheet Design:** Designing a process flowsheet is a critical milestone of a chemical process plant design. The rationale underlying this fact is that the process flowsheet provides the big picture of the material and energy flow within the process, process steps, and equipment used to carry out each step, such as reaction, heating, cooling, separation, purification, and product storage in tanks and receivers.

Fig. 1.10 represents an excerpt from a process flowsheet, where a reactor outlet stream at a high temperature is cooled down first. This stream is now a two-phase flow material stream, which should be split into liquid and gas streams in a flash drum for transportation by a pump (for the liquid phase) and a compressor (for the gas phase).

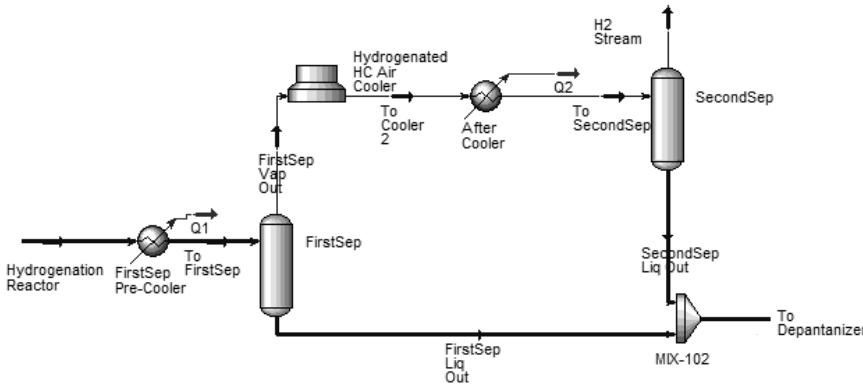



**Fig. 1.10** The PFD of a cooling and phase separation section; Aspen HYSYS.

There are many essential steps to designing an ideal process flowsheet and making the designed chemical process inherently safe and environmentally friendly. Process engineers may use process design software, such as Aspen HYSYS, Aspen Plus, PRO II, and CHEMCAD, to generate or modify several process flowsheets for manufacturing a single product and choose the best process among design arrays.

**G. Heat and Material Balance:** One of the incredible abilities of a process simulator is generating a table of Heat & Materials (H & M) balance. When a chemical engineer designs a process flowsheet using process simulators, the simulators generate H & M balance tables.