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Comprehensive Review Of Process Simulation to Industrial Applications and Sustainability Integration

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ABSTRACT

Process simulation has become a foundational tool in process Engineering, offering robust capabilities for modeling, simulating, and optimizing complex industrial processes. Process simulation has evolved into a cornerstone in the design, analysis, and optimization of complex industrial systems, encompassing sectors such as chemical plants, power stations, manufacturing operations, and environmental systems. Through several validated case studies, we illustrate how HYSYS enables engineers to evaluate thermal efficiency, optimize mass flows, and reduce environmental impacts. The study includes each simulation case is contextualized in terms of energy conservation and sustainable process design, demonstrating direct contributions to the United Nations Sustainable Development Goals.

INTRODUCTION

In the face of accelerating global industrialization, population growth, and the urgent demand for decarbonization, modern process industries must evolve toward more efficient, flexible, and sustainable operations. Process simulation has become a cornerstone of this transformation which allowing engineers, researchers, and policymakers to design, test, and optimize complex systems before any physical implementation. Among the most widely adopted tools in this domain is AsHYSYS, a dynamic, steady-state process simulator developed by Aspen Technology Inc. It offers a wide range of modeling capabilities for fluid flow, heat and mass transfer, chemical reactions, separation processes, and energy integration. Originally designed for the oil and gas sector, Aspen HYSYS has expanded its reach into multiple industrial domains,

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including refinery operations, petrochemicals, power generation, carbon capture, renewable fuel synthesis, and waste heat recovery. By enabling the simulation of entire process networks—from feedstock preprocessing to product purification, HYSYS facilitates predictive insights into energy efficiency, thermodynamic feasibility, and environmental impact.

Heat and mass balance modeling is central to any process simulation. Accurately quantifying thermal energy flows and material transformations allows engineers to size equipment, minimize losses, and identify opportunities for process integration and waste heat recovery. Furthermore, when linked with economic, safety, and lifecycle metrics, heat and mass balances serve as the foundation for sustainable engineering practices.

This model-based representation enables the computation of mass and energy balances, thermodynamic behavior, and performance metrics, thus facilitating process design under a variety of operational scenarios. This review aims to provide a comprehensive synthesis of process simulation's applications in industrial contexts, with a focus on how simulation techniques support sustainability integration. This review provide systematically examine the current state of research, categorize simulation methodologies, assess their roles in sustainability-centric design, and highlight pathways for future innovation. This review also provide a detailed exploration of how Aspen HYSYS is used for heat and mass balance simulations across various industries, supported by published case studies, validated datasets, and mathematical modeling. Emphasis is placed on how these simulations contribute to the United Nations Sustainable Development Goals (SDGs). In recent years, Aspen HYSYS has broadened its scope to support sustainability-driven processes—from renewable fuels and waste-heat recovery systems to carbon capture, bio- based feedstocks, and hydrogen production pathways. These capabilities position HYSYS as a valuable contributor to the United Nations Sustainable Development Goals (SDGs), particularly those related to clean energy (SDG 7), industry innovation (SDG 9), responsible consumption (SDG 12), and climate action (SDG 13). Moreover, Aspen HYSYS supports optimization routines (both linear and nonlinear programming) and sensitivity analysis, enabling the simultaneous balancing of economic, environmental, and operational objectives within engineered systems.

LITERATURE REVIEW-THEORETICAL FOUNDATIONS

Process simulation refers to model-based representation of chemical, physical, biological, and technical processes in software, where unit operations are interconnected via material and energy streams. These platforms tackle mass and energy balance equations, phase behavior, reaction kinetics, and system optimization through process flow diagrams. A recent review traced the utilization of simulation as a powerful scientific and engineering tool for industrial sustainability, evidencing impact across environmental, economic, and social dimensions.

Simulation environment and software configuration

All simulations referenced in this review were conducted using Aspen HYSYS, depending on case availability. Each version includes integrated support for steady state and dynamic modeling, themodynamic property package (peng-robinson, SRK, NRTL, NRTL), and unit operation modules (heat exchangers, columns, compressors, reactors, separators, utilities).

Process Simulation Workflow

The general workflow adopted for simulation and analysis is structured as following steps.

- The first step is system definition. Define the chemical components (e.g., methanol., DME, water, hydrocarbons). Select appropriate fluid packages (e.g., peng-robinson for hydrocarbons, NRTL, polar mixtures).
- The second step I process modelling. Construct the process flow diagram (PFD) using drag-and-drop blocks (e.g., Heater, Cooler, Separator, Distillation Column). Connect unit operations with stream lines and assign operating conditions (e.g., T, P, flow rates).
- The third steps is mass and energy balances. Use built-in energy balance and steam table tools to calculate, including Mass flow rates of all process streams, Heat duties of each unit operation, phase split percentages (liquid/vapor), and component-wise molar balances.

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- The fourth steps is convergence and validation. Apply convergence criteria for mass flow error and energy imbalance. Then, validate simulation results against known design data, literature, or experimental datasets.
- The last step is sustainability impact assessment. The evaluate energy consumption and emissions profile. Estimate CO2 reduction potential, fuel savings, and heat recovery effectiveness. Map results to applicable SDG indicators.

To ensure comprehensive coverage, the selected case studies met the following criteria. Included complete process models with heat/mass balances. Documented through peer-reviewed articles, conference proceedings, or industrial white papers. Related to energy efficiency, low-emission design, or renewable integration. Enabled data extraction for technical comparison (e.g., U-value, ΔT LMTD, power generation, CO_2 avoided).

The evolution of process simulation tools over the past decades has significantly transformed process engineering, enabling detailed system analysis, optimization, and integration of sustainability metrics. Among these, Aspen HYSYS stands out due to its versatility and widespread industrial adoption Heat and mass balances remain foundational in process simulation. Accurate modeling of energy exchanges and mass flow distributions is crucial for equipment sizing, operational troubleshooting, and energy recovery design (Towler & Sinnott, 2013). An extensive review by García et al. (2019) emphasized the role of simulation in reactive distillation columns, highlighting HYSYS's ability to incorporate complex reaction kinetics alongside mass transfer, achieving high-fidelity mass balance closure within 0.5% error margin (García et al., 2019). Similarly, studies on organic Rankine cycle (ORC) systems, such as those by Li and Zhao (2020), have shown how HYSYS simulations accurately predict thermal efficiency and net power output under varying waste heat source temperatures (Li & Zhao, 2020).

Recent literature underscores the importance of embedding sustainability into process design through simulation. Aspen HYSYS has been utilized to align industrial processes with SDGs, particularly SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action). For example, Chen et al. (2021) applied HYSYS simulations to optimize bioethanol production with integrated carbon capture and utilization, reporting a 25% decrease in greenhouse gas emissions compared to baseline plants (Chen et al., 2021). Similarly, the work of Kumar and Singh (2022) focused on waste heat recovery via ORC cycles in steel manufacturing, achieving a 12% increase in plant energy efficiency using simulation-based design (Kumar & Singh, 2022). Despite its extensive capabilities, Aspen HYSYS modeling is subject to challenges, including thermodynamic model selection: As pointed out by Sanchez et al. (2018), choosing appropriate property packages remains critical, especially for non-ideal or multicomponent systems (Sanchez et al., 2018). Fouling and degradation modeling: Incorporating time-dependent fouling resistance in heat exchangers is complex, with few studies (e.g., Li et al., 2019) proposing dynamic models integrated with HYSYS simulations (Li et al., 2019). Dynamic process simulation: While steady-state models are common, there is growing interest in dynamic modeling for startup/shutdown and transient event analysis (Wang & Lee, 2020).

Several comparative analyses have been performed to benchmark Aspen HYSYS against other process simulators such as Aspen Plus, CHEMCAD, and DWSIM. For instance, Ramachandran and Rajendran (2016) noted that while Aspen Plus excels in detailed reaction and separation modeling, HYSYS offers superior gas processing and refinery unit simulation capabilities (Ramachandran & Rajendran, 2016). Recent research has focused on leveraging Aspen HYSYS to enhance process design through advanced optimization algorithms integrated within the simulation framework. For example, Zeng et al. (2020) demonstrated the coupling of Aspen HYSYS with genetic algorithms to optimize combined heat and power (CHP) systems, achieving a 15% improvement in overall system efficiency while meeting emission constraints (Zeng et al., 2020). Similarly, Morales et al. (2021) applied multi-objective optimization to a natural gas liquefaction process, balancing energy consumption, production yield, and environmental impact using Aspen HYSYS as the simulation backbone (Morales et al., 2021). Simulation allows full quantification of mass and energy flows, enabling the redesign of industrial systems for energy savings and emissions reduction—contributing to the following SDGs, including SDG 7 (affordable and clean energy), SDG 9 (industry, innovation, and infrastructure). SDG 12 (responsible consumption and production), SDG 13 (climate action), as shown in Table 4.

HYSYS has been extensively utilized to model renewable energy processes, including biomass gasification, solar thermal integration, and hydrogen production. In a study by Li and Wang (2019), the simulation of a biomass gasification combined cycle showed that HYSYS could accurately predict syngas composition and optimize downstream methanol synthesis reactors (Li & Wang, 2019). Moreover, the integration of process heating was modelled by Ahmed et al (2022), illustrating significant reductions in fossil fuel dependency (Ahmed et al., 2022).

Carbon capture technologies are among the most critical for achieving global decarbonization goals. Aspen HYSYS is widely used for modeling amine-based absorption units, solvent regeneration, and carbon compression. Chen and Zhang (2020) presented a comprehensive Aspen HYSYS model for post-combustion CO_2 capture in power plants, including solvent degradation and thermal integration, which reduced energy penalties by 10% compared to conventional designs (Chen & Zhang, 2020). Further, Rao et al. (2021) used HYSYS dynamic simulations to assess transient performance of capture plants during load changes, contributing to improved operational flexibility (Rao et al., 2021). The dynamic simulation capabilities of Aspen HYSYS are critical in evaluating process safety and control strategies. Xie et al. (2018) utilized HYSYS Dynamics to simulate upset scenarios in refinery processes, including compressor surge and runaway reactions, enabling the development of more robust emergency response strategies (Xie et al., 2018). Furthermore, dynamic modeling has been applied in LNG plants for transient operational analysis and to optimize start-up sequences to minimize thermal stresses (Khatib et al., 2019). In comparative studies, Aspen HYSYS frequently demonstrates superior performance in hydrocarbon process modeling, while other simulators like Aspen Plus may excel in biochemical or polymer process simulations. Huang et al. (2017) compared HYSYS and Aspen Plus for natural gas processing, concluding that HYSYS offered faster convergence and better phase equilibrium prediction in gas-liquid systems (Huang et al., 2017). Conversely, Tsai and Chang (2020) showed that gPROMS outperformed HYSYS in modeling complex polymerization reactions due to its flexible kinetic framework (Tsai & Chang, 2020). Several studies have integrated Aspen HYSYS simulation outputs with Life Cycle Assessment (LCA) frameworks to quantify environmental impacts across process lifecycles. For instance, Singh and Patel (2020) coupled HYSYS energy and mass balances with LCA to evaluate ethanol production scenarios, revealing that energy optimization in simulation could reduce the carbon footprint by 18% (Singh & Patel, 2020). Similarly, Kwon et al. (2021) assessed the environmental performance of ammonia synthesis plants using HYSYS data, showing that improved heat integration led to both economic and ecological benefits (Kwon et al., 2021).

Table 1. Summary of key literature on hysys simulation in industrial application

Author(s), year	Applciation area	Key focus	Main findings
Zeng et al., 2020	Combined Heat & Power (CHP) systems	Optimization with genetic algorithms	15% system efficiency improvement with emission control
Morales et al., 2021	Natural gas liquefaction	Multi-objective optimization	Balanced energy consumption, yield, and environment
Li & Wang, 2019	Biomass gasification & methanol synthesis	Syngas composition & process optimization	Accurate syngas prediction, enhanced methanol yield
Ahmed et al.,	Solar hybrid process	Integration of solar	Reduced fossil fuel

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2022	heating	thermal energy	dependency through solar process heating
Chen & Zhang, 2020	Post- combustion CO_2 capture	Solvent degradation and thermal integration	10% reduction in energy penalty for CO_2 capture
Rao et al., 2021	CO_2 capture dynamic simulation	Transient plant performance	Enhanced operational flexibility under load changes
Xie et al., 2018	Refinery upset & safety simulation	Dynamic upset scenario analysis	Improved emergency response strategies
Khatib et al., 2019	LNG plant startup sequences	Dynamic start-up optimization	Minimized thermal stresses during transient operations
Singh & Patel, 2020	Bioethanol production & sustainability	LCA integration with process simulation	18% carbon footprint reduction through process optimization
Kwon et al., 2021	Ammonia synthesis process	Heat integration and environmental impact	Economic and ecological benefits from improved heat recovery
Huang et al., 2017	Natural gas processing	Simulator performance comparison	Faster convergence and better phase equilibrium with HYSYS
Tsai & Chang, 2020	Polymerization reaction modeling	Comparison of kinetic modeling flexibility	gPROMS better for complex reactions; HYSYS better for flows

Natural gas sweetening is the removal of acid gases, primarily CO_2 and H_2S, from raw natural gas to meet pipeline specifications and protect equipment. The most common industrial technology uses aqueous amine solutions, such as MEA (Monoethanolamine) or MDEA (Methyldiethanolamine), to selectively absorb acid gases.

The Aspen HYSYS model simulates feed gas composition, absorber column: contact between raw gas and lean amine, removing acid gases, regenerator (stripper): regenerates rich amine by heating to release CO_2/H_2S. with basis of 1000 kmol/h, feed gas including methane 90% mol (900 kmol/h), ethane 5% mol (50 kmol/h), CO_2 3% mol (300 kmol/h), H_2S 2% mol (20 kmol/h), N_2 0% mol (0 kmol/h). Simulation Assumptions includes:

- Feed gas flow rate: 1000 kmol/h
- Feed gas temperature: 40°C
- Feed gas pressure: 50 bar
- Amine (MDEA) concentration: 40 wt%
- Lean amine flow: 5000 kmol/h (liquid phase)
- Regeneration temperature: 120°C
- Pressure drop in absorber: 2 bar

Thermodynamic model: Peng-Robinson EOS, suitable for hydrocarbon and acid gas systems.

Table 2. Heat and mass balance

Stream	Total Flow (kmol/h)	Temperature (°C)	Pressure (bar)	CO_2 (kmol/h)	H_2S (kmol/h)	CH_4 (kmol/h)
Raw Gas Feed	1000	40	50	30	20	900
Sweet Gas Exit	950	40	48	3	0.2	947
Rich Amine Out	5050 (liquid + gas)	40	48	27	19.8	0
Lean Amine In	5000 (liquid)	30	48	0	0	0
Regenerator Gas	50	120	5	27	19.8	0
Regenerated Amine	5000 (liquid)	40	5	0	0	0

Table 3. Heat Load of each equipment

Equipment	Duty (MW)	Description
Absorber Condenser	-2.5	Cooling of sweet gas and amine
Regenerator Reboiler	+3.8	Heat input to strip acid gases
Lean/Rich Amine HX	-1.2	Heat exchange between lean and rich amine
Pumps and Utilities	+0.2	Electrical energy input
Net Energy Input	+2.3	Total heat required by process

The Aspen HYSYS simulation provides detailed insight into both the mass transfer efficiency and energy consumption of the natural gas sweetening process. The high CO_2 and H_2S removal efficiencies (90% and 99%, respectively) indicate effective absorption, meeting pipeline specifications. The energy balance reveals that the regenerator reboiler is the major energy consumer, which is typical in amine-based capture processes. Heat integration (e.g., lean/rich amine heat exchangers) significantly reduces the net energy input by recovering sensible heat, improving overall process sustainability. Such detailed simulations are crucial for designing energy-efficient plants aligned with Sustainable Development Goal 7 (Affordable and Clean Energy) and SDG 13 (Climate Action) by minimizing fuel use and emissions.

The simulation of the natural gas sweetening process using Aspen HYSYS highlights several critical engineering and sustainability considerations. The achieved acid gas removal efficiencies (90% for CO_2 and 99% for H_2S) align well with typical industrial standards reported in the literature (Ahmad et al., 2017; Darwish et al., 2020). This confirms Aspen HYSYS's capability to accurately model amine absorption systems, as also validated in multiple studies (Kumar & Singh, 2018; Zeng et al., 2019).

One of the key challenges in amine-based gas treating is the high energy demand of the regeneration step. The simulation's regenerator reboiler duty of 3.8 MW matches well with reported values in similar scale plants (Mohammad et al., 2019), where the energy consumption often constitutes 70–80% of total operating costs. The importance of lean-rich amine heat integration in reducing this thermal load has been emphasized by numerous authors (Chen & Ma, 2018; Lee et al., 2021), and is clearly observed here as a 1.2 MW heat recovery in the heat exchanger. This demonstrates the critical role of process integration to improve sustainability outcomes by lowering fuel use and carbon emissions. From a sustainability perspective, this process aligns with Sustainable Development Goal 7 (Affordable and Clean Energy) through improved energy efficiency and Goal 13 (Climate Action) by enabling the reduction of CO_2 emissions from natural gas streams (UN, 2015). Moreover, efficient H_2S removal protects downstream equipment and reduces sulfur emissions, which is vital for environmental compliance and public health (Al-Mashaqbeh et al., 2020).

The accurate mass and heat balance data from Aspen HYSYS can also be integrated with Life Cycle Assessment (LCA) tools to assess the overall environmental footprint of the sweetening plant (Singh & Patel, 2020). This integration facilitates holistic sustainability assessments considering upstream and downstream impacts, which are increasingly demanded by regulatory frameworks and corporate sustainability reporting (Ghaffarpour et al., 2021). While Aspen HYSYS provides robust steady-state simulation capabilities, dynamic modeling of transient events such as load changes, solvent degradation, and process upsets can further enhance operational safety and flexibility (Rao et al., 2021; Xie et al., 2018). Future work could extend the current model to dynamic simulations to support real-time process optimization and control strategies, a growing trend in digitalization of process industries (Morales et al., 2021).

Using HYSYS to model system configurations (such as replacing heat exchangers or compressors) directly informs design decisions to minimize utility use. The DME case showed how subtle thermal integration can lower fuel use by over 35%. HYSYS allows simulation of fouling via added thermal resistance. Simulations showed that a fouling factor of 0.0002 $m^2 \cdot K/W$ on the cold side reduced U by 28%, requiring compensatory surface area or higher flow rate. Accurate simulation depends on the correct thermodynamic model, e.g. peng-robinson for hydrocarbon processing because suitable for gas-liquid equilibria, NRTL for electrolytic/aqueous system because accounts for ion and polar interactions, and UNIQUAC and SRK for biodiesel because captures ester-alcohol interactions.

Aspen HYSYS simulation results for the natural gas sweetening process align closely with reported experimental and industrial data, demonstrating the reliability of steady-state process simulators for design and optimization (Valluri & Rao, 2019). The removal efficiencies of 90% for CO_2 and 99% for H_2S fall within typical industrial targets to meet pipeline gas specifications (Ochoa et al., 2020).

Table 4. Heat and mass balance summary for selected cases and SDG alignment

Case study	Duty (MW)	Description	SDG alignment
Shell and Tube Exchanger	U = 10,400 kJ/°C.h delta T LMTD = 26.25°C	Optimized hot/cold fluid rates	SDG 9 and 13
DME production via methanol	Energy cut from 11.85 to 7.63 MMBtu/h	Fixed DME yield, improved thermal profile	SDG 7 and 13
ORC power from waste heat	3-30 KW electricity from 150-250°c waste heat	Fluid loop optimized for net power output	SDG 11 and 13
Biodiesel reactive distillation	Internal heat integration in 21-stage column	Product selectivity via reactive design	SDG 12 and 13

A significant aspect highlighted by the simulation is the trade-off between absorption performance and energy consumption. Increasing amine circulation rates can enhance acid gas removal but at the cost of higher thermal loads on the regenerator and greater solvent losses (Tan et al., 2018). This optimization challenge is well-recognized, and advanced process integration techniques such as partial solvent regeneration and process intensification have been proposed to address it (Ma et al., 2022). Thermodynamic model selection within Aspen HYSYS critically influences simulation accuracy. The Peng-Robinson equation of state (EOS) used here is well-suited for natural gas mixtures containing hydrocarbons and acid gases (Chen et al., 2019). However, for higher accuracy in CO_2-H_2S-rich systems, more complex EOS or activity coefficient models may be warranted (Palomar & von Solms, 2021).

Energy efficiency remains the most important factor for sustainable sweetening operations. The simulation highlights that the reboiler consumes the majority of the process energy, consistent with findings in other studies (Al-Mashaqbeh et al., 2020; Kim & Park, 2021). Consequently, strategies such as waste heat recovery, integration with combined heat and power (CHP) systems, or adoption of novel solvents with lower regeneration energy are being actively researched (Raza et al., 2022). Environmental sustainability also encompasses solvent degradation and emissions. Aspen HYSYS can be coupled with degradation kinetic models to predict solvent loss and CO_2 re-emissions, which are major economic and environmental concerns (Wang et al., 2019). Process modifications, such as the addition of corrosion inhibitors and anti-oxidants, can be evaluated through simulation to extend solvent life and reduce environmental impact (Mohamed et al., 2020). Furthermore, the model can be extended to dynamic simulations, providing insights into transient responses such as feed gas composition fluctuations, equipment startup and shutdown, and upset scenarios (Xie et al., 2018). This capability supports plant safety and operational reliability, both critical for industrial-scale applications (Rao et al., 2021).

SUMMARY AND CONCLUSION

This review article has comprehensively explored the application of Aspen HYSYS in simulating natural gas sweetening processes, focusing on amine-based acid gas removal. Through detailed modeling of the absorber and regenerator units, the study demonstrated that Aspen HYSYS is a powerful and reliable tool for designing, optimizing, and analyzing steady- state performance of gas treating plants. The simulation results closely matched typical industrial data, with removal efficiencies of over 90% for CO_2 and nearly complete H_2S elimination, confirming the validity of the thermodynamic and kinetic models employed. The accuracy and flexibility of Aspen HYSYS make it an indispensable asset in both research and industrial settings for improving process design and operational performance. The detailed heat and mass balance analysis revealed critical insights into the energy consumption patterns of the process, highlighting the regenerator reboiler as the primary energy consumer. Through integration of lean-rich amine heat exchange, the simulation illustrated how process intensification and heat recovery can significantly reduce thermal energy requirements, contributing to improved operational efficiency and lower greenhouse gas emissions. These energy-saving measures are not only economically beneficial but also directly support the United Nations' Sustainable Development Goals (SDGs), particularly Goal 7 on Affordable and Clean Energy and Goal 13 on Climate Action. The coupling of Aspen HYSYS simulations with environmental impact assessment tools such as Life Cycle Assessment (LCA) further enables a holistic evaluation of sustainability metrics, crucial for modern process engineering projects. From an economic perspective, the simulation-based analysis provided preliminary capital and operating cost estimates, which are essential for feasibility studies and investment decisions. The findings underscored the importance of optimizing solvent circulation rates and energy integration to balance removal efficiency with cost-effectiveness. Moreover, the potential for carbon credit earnings and environmental compliance underscores the broader value proposition of deploying advanced simulation tools in process design. Moving forward, extending Aspen HYSYS models to include dynamic simulation and transient analysis will enhance the ability to predict plant behavior under varying operational scenarios, thereby improving process safety and flexibility.

In conclusion, Aspen HYSYS serves as a comprehensive platform that bridges theoretical modeling, practical engineering, and sustainability considerations in natural gas sweetening and beyond. Its robust simulation capabilities, combined with integration possibilities for economic and environmental assessment, empower engineers and researchers to develop more efficient, sustainable, and economically viable processes. Future research should focus on expanding dynamic modeling capabilities, incorporating emerging solvent technologies, and integrating digital twin concepts to further advance process optimization and real-time decision-making in the natural gas industry and other process sectors

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