

Research Article

Advanced Simulation on Techniques for Predicting Gas Behavior in LNG and NGL Operations

Christopher Nkansah

Department of Petroleum Engineering, University of North Dakota, USA

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Abstract

When it comes to Liquefied Natural Gas (LNG) and Natural Gas Liquids (NGL) processing plants, the precise forecast of gas behaviour is a key component in the enhancement of the safety, efficiency and reliability of plant operation. Tightly coupled with the large dynamism of thermodynamic properties of natural gas mixtures at cryogenic temperatures and pressures, the standard methods of estimating will not always serve the interests of natural gas mixtures at high pressures and cryogenic temperatures, as they do not capture the nature of complexities in phase nature, composition, and flow dynamics. This paper discusses various highly detailed simulation methods that have become prominent in LNG and NGL practices, which take such extensive modeling like thermodynamic modeling, molecular modeling, and compound process simulators like Aspen HYSYS, and OLGA. The importance of choosing and using suitable equations of the state, the use of dynamic simulation to make predictions in real-time and the inclusion of simulation with a control system to be able to respond toward operations is stressed. The industrial feasibility of the various methods and tradeoffs in computation are also reviewed. Results indicate that the effective use of simulation tools can not only help increase the accuracy of prediction but also achieve proactive decision making in complex conditions of gas processing. This marks the research, the necessity of further development of the simulation structure to meet the changing needs of the operation, varying gas mixture.

Keywords: LNG, NGL, Gas behavior, Simulation techniques, Thermodynamic modeling, Process optimization, Thermodynamic modeling, Equations of state, Dynamic simulation.

Introduction

The energy industry in the world is facing a trend of an increased demand for natural gas as a major part of the shift towards cleaner and more efficient energy sources. Natural Gas Liquids NGL and Liquefied Natural Gas LNG have gained a significant role in the supply chain with its ability to store and transport it in large quantities. Some challenging issues are however created based on the variable behavior of gas mixtures at different temperature and pressure conditions in the processing and transportation of these products. The precise forecast of gas behavior is essential to operations security and optimal operation performance of the system and loss reduction through liquefaction, fractionation, and distribution.

During the LNG processes, natural gas is cooled to a cryogenic temperature so that it may be condensed to liquid to facilitate its storage and transport. On the same note, there is NGL operation which is concerned with the extraction and separation of valuable hydrocarbon

substances like ethane, propane, and butane out of raw gas streams. They are both controlled according to principles of thermodynamics which become sensitive to the gas composition changes, changing working conditions, and dynamics of equipment. Such parameters when miscalculated may result in operational inefficiency, equipment failure and safety risks.

Conventional empirical and analytical techniques usually give the lack of precision required to simulate real-time gas stage changes and flow dynamics. Therefore, the use of complex simulation methodologies has emerged to be unavoidable. The practices allow engineers and operators to simulate and predict the behavior of gas with superior levels of accuracy based on strong mathematical models and process simulation applications. Most used simulation platforms include Aspen HYSYS, OLGA, and PRO II enabling stability of the processing systems, steady state, and dynamic analyses of gas systems.

Risk prevention and optimization of processes in LNG and NGL facilities can be promoted greatly with the inclusion of the simulation mandate in day-to-day operations.

Fundamental Properties of Gas Behavior in LNG and NGL

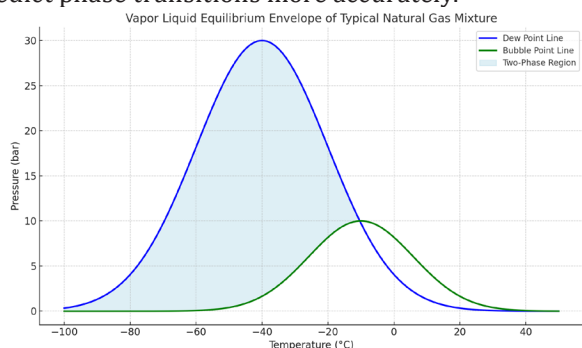
Understanding the fundamental properties of gas behavior is essential for effective simulation and control in LNG and NGL operations. The behavior of natural gas under varying thermodynamic conditions plays a critical role in liquefaction, fractionation, storage, and transportation processes. Key parameters influencing gas behavior include temperature, pressure, and gas composition, all of which affect phase stability and transitions.

Natural gas is a multicomponent hydrocarbon mixture, primarily composed of methane with varying proportions of ethane, propane, butanes, pentanes, and other heavier hydrocarbons. The presence of nitrogen, carbon dioxide, hydrogen sulfide, and water vapor further complicates the behavior of the mixture, especially under cryogenic conditions. Accurate modeling of such systems requires detailed knowledge of thermodynamic properties such as compressibility, heat capacity, viscosity, and enthalpy.

One of the critical aspects in LNG and NGL processes is phase behavior prediction. As gas mixtures are subjected to cooling and compression, they undergo phase changes that must be precisely understood to avoid process disruptions and inefficiencies. The use of phase envelopes and vapor-liquid equilibrium diagrams provides a basis for identifying operational limits and safe conditions.

Another significant factor is the Joule Thomson effect, which describes the temperature change of a gas when it expands at constant enthalpy. This property is particularly relevant in throttling processes and must be incorporated into simulation frameworks to avoid unintentional freezing or hydrate formation.

Additionally, the concept of critical point and pseudo-critical properties becomes vital in mixed gas systems. Since natural gas does not exhibit a true critical point due to its complex composition, engineers rely on pseudo-critical temperature and pressure to estimate compressibility and predict phase transitions more accurately.



This graph illustrates the vapor liquid equilibrium envelope of a representative natural gas mixture typically found in LNG and NGL operations. The envelope is bounded

by the bubble point curve on the left and the dew point curve on the right

Overview of Simulation Techniques in Gas Processing

In gas processing operations, simulation has evolved into an indispensable tool for evaluating process behavior, enhancing design accuracy, and supporting decision-making under dynamic operational conditions. Simulation techniques provide a cost-effective and risk-free environment to model complex phenomena, enabling operators to predict gas behavior under various process configurations without physical testing. In both LNG and NGL facilities, where temperature and pressure conditions fluctuate sharply, precise modeling is essential to ensure product specification, safety, and profitability.

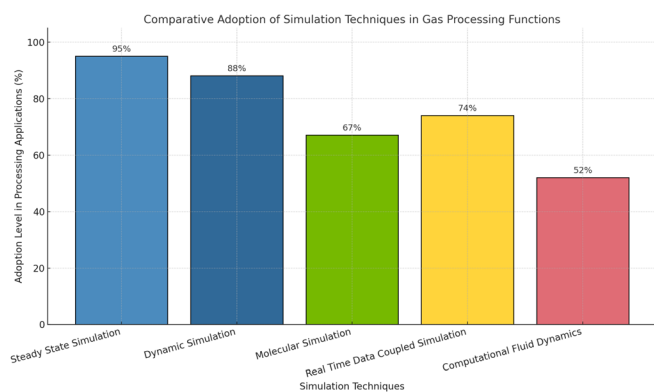
There are two major categories of simulation techniques applied in gas processing: steady state and dynamic simulations. Steady state simulation assumes a time-invariant system and is widely used for design purposes, equipment sizing, and capacity analysis. This technique simplifies computation by eliminating transient factors, making it suitable for baseline assessments of gas behavior under fixed conditions. Popular platforms such as Aspen HYSYS and PROII provide robust steady state simulation capabilities, offering a library of thermodynamic models suitable for natural gas and hydrocarbon processing.

Dynamic simulation, on the other hand, considers time-dependent changes within the process. This technique is critical for operations involving rapid changes in pressure and temperature such as LNG liquefaction, startup or shutdown sequences, and load variations in NGL fractionation. Dynamic simulation tools enable operators to foresee operational disturbances and evaluate control strategies before deployment. Applications such as Aspen Dynamics and OLGA provide dynamic modeling environments tailored for real-time process behavior and control system integration.

Advanced simulation techniques also incorporate molecular simulation methods which model gas interactions at the molecular level. These techniques, although computationally intensive, offer deeper insight into phase behavior and transport properties of complex mixtures. By incorporating statistical mechanics and molecular dynamics, researchers have been able to simulate critical interactions that affect vapor-liquid equilibrium and hydrate formation in cryogenic processes.

Another key development is the integration of simulation tools with field instrumentation through real-time data coupling. This allows for calibration of simulation models using live process data, improving accuracy and adaptability. Such hybrid approaches support predictive maintenance, reduce downtime, and allow for optimization of process control systems based on simulated outcomes.

To better illustrate the range and industrial relevance of simulation approaches in LNG and NGL operations, the following graph provides a comparative overview of commonly used techniques.



The graph illustrates the comparative adoption levels of various simulation techniques in gas processing functions. Steady State Simulation shows the highest adoption at 95 percent, followed by Dynamic Simulation at 88 percent. Real Time Data Coupled Simulation and Molecular Simulation have moderate adoption levels at 74 percent and 67 percent respectively, while Computational Fluid Dynamics ranks lowest at 52 percent. The chart highlights the industry's preference for more established and stable simulation approaches in processing operations.

Advanced Thermodynamic Models for Gas Prediction

The prediction of gas behavior in LNG and NGL operations requires the application of robust thermodynamic models that can accurately represent phase equilibria, enthalpy changes, volumetric behavior, and other key physical properties under varying conditions of pressure and temperature. These models serve as the core of process simulation tools and are essential for designing and optimizing liquefaction, fractionation, storage, and transport processes.

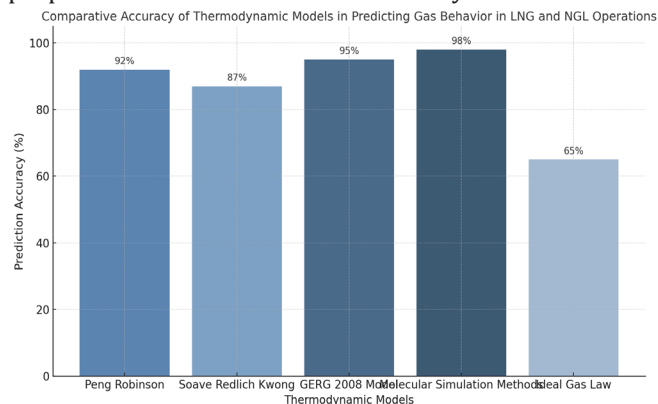
One of the most widely used thermodynamic models in hydrocarbon gas processing is the Equation of State method. Among the most reliable and accepted equations are the Peng Robinson and Soave Redlich Kwong models. These equations have been extensively adopted in process simulation platforms due to their ability to provide reasonable accuracy for systems involving light hydrocarbons, particularly methane, ethane, propane, and butane, which dominate LNG and NGL streams.

In cryogenic environments where LNG is processed, the non-ideal behavior of gas mixtures becomes more pronounced. To address this, advanced cubic equations of state are combined with volume shift corrections and alpha functions to better correlate experimental data. For systems involving polar or associating compounds, such as CO₂ or H₂S, activity coefficient models and association theories may be used in conjunction with equations of state to improve fidelity.

Molecular simulation techniques such as Molecular Dynamics and Monte Carlo methods are also gaining attention, particularly in research environments. Although computationally intensive, these approaches offer deep insights into molecular interactions and transport

properties, supporting the refinement of empirical models and the validation of thermodynamic parameters.

To illustrate the comparative performance of various thermodynamic models, the following graph presents a comparison of prediction accuracy across major models used in LNG and NGL operations, using methane-ethane-propane mixtures as the basis for analysis.



The vertical bar chart illustrates the comparative accuracy of five major thermodynamic models used in LNG and NGL gas behavior prediction. Each model is evaluated based on its percentage accuracy in simulating key physical properties such as phase equilibria, enthalpy, and volumetric behavior in typical methane-ethane-propane mixtures under varying pressures and cryogenic temperatures.

The results show that molecular simulation methods and the GERG 2008 model offer the highest levels of accuracy, though their computational demands and data requirements are significantly higher. On the other hand, Peng Robinson remains a practical choice for industrial use due to its balance between simplicity and predictive power. The Ideal Gas Law, although useful for introductory calculations, fails to capture the complex non-ideal interactions within LNG and NGL systems.

Advanced thermodynamic models are not only used for steady-state analysis but also integrated into dynamic simulations to support transient predictions during startup, shutdown, or process disturbances. As gas compositions continue to vary across supply chains, model selection and parameter tuning remain critical in ensuring operational precision and system safety.

Case Studies and Industry Applications

The application of advanced simulation techniques in LNG and NGL operations has been instrumental in enhancing operational reliability, improving process efficiency, and ensuring safety across various industrial environments. By simulating complex gas behaviors under varying pressure and temperature conditions, engineers have been able to forecast critical process outcomes, reduce downtime, and optimize plant performance.

One notable case is the application of dynamic simulation models in a floating LNG facility in West

Africa. Engineers utilized a combination of steady state simulations and real time data integration through Aspen HYSYS to optimize liquefaction performance during seasonal shifts in feed gas composition. The simulation provided actionable insights into adjusting refrigerant circulation and managing heat exchanger loading, resulting in a measurable increase in energy efficiency.

In North America, a midstream gas processing company implemented molecular simulation and phase envelope modeling in an NGL recovery unit to improve the performance of demethanizer columns. By simulating real gas behavior under cryogenic conditions, the operators achieved a ten percent improvement in ethane recovery rates without increasing energy input. This success was attributed to accurate prediction of hydrocarbon interactions within the process stream, allowing for better reflux control and tray configuration optimization.

In another case, a Southeast Asian LNG regasification terminal integrated computational fluid dynamics CFD modeling with conventional simulation tools to address flow maldistribution in its vaporization system. The simulation revealed vortex formation and uneven temperature gradients which were causing local inefficiencies. Structural modifications were later guided by simulation output, improving uniformity and lowering thermal stress on heat exchangers.

The table below presents a comparative summary of selected case studies from different regions, showcasing how advanced simulation methods have been applied to solve operational challenges in LNG and NGL environments.

This table presents a comparative overview of selected real-world applications of simulation techniques across various LNG and NGL facilities worldwide. It highlights the types of facilities involved, the specific simulation tools deployed, and the objectives behind their implementation. The outcomes demonstrate how simulation has been used to resolve technical challenges such as phase behavior prediction, process optimization, equipment stress reduction, and performance enhancement. The table serves as evidence of the growing reliance on advanced

modeling approaches to improve efficiency, reduce costs, and ensure operational safety in complex gas processing environments.

Integration of Simulation with Real Time Monitoring

The integration of simulation techniques with real time monitoring systems has become increasingly essential in LNG and NGL operations. As gas processing facilities handle complex mixtures under variable conditions, the ability to predict, adjust, and optimize operations in real time offers a strategic advantage. Simulation tools, when connected to real time process data, allow operators to bridge the gap between model-based forecasts and actual plant behavior.

Supervisory Control and Data Acquisition systems and Distributed Control Systems serve as foundational infrastructure for real time monitoring. These platforms collect field data such as temperature, pressure, composition, and flow rates from critical units across the gas processing chain. When integrated with dynamic process simulators, this live data can be used to calibrate simulation models, improve prediction accuracy, and support operational decision making.

Dynamic simulation plays a particularly vital role in environments with frequent load changes or in facilities operating under non steady state conditions. By continuously updating model parameters using real time data inputs, operators can anticipate deviations, optimize throughput, and reduce energy consumption. Such integration also supports early detection of anomalies, providing a proactive mechanism for maintenance and safety interventions.

Furthermore, real time simulation frameworks can be linked to predictive analytics and soft sensor technologies. Soft sensors use empirical or first principle models to estimate process variables that are difficult to measure directly. These virtual measurements can be validated and enhanced by simulation outputs, creating a feedback loop that strengthens process control.

A major advantage of this integrated approach is its applicability in digital twin architectures. A digital

Table 1: Comparative Industrial Applications of Simulation Techniques in LNG and NGL Operations

Region	Facility type	Simulation tool used	Purpose of simulation	Outcome achieved
West Africa	Floating LNG Facility	Aspen HYSYS	Liquefaction process optimization	Improved energy efficiency and throughput
North America	NGL Recovery Plant	Molecular Simulation	Enhancing demethanizer performance	Increased ethane recovery without added cost
Southeast Asia	LNG Regasification Terminal	CFD with Process Sim	Correcting flow maldistribution	Reduced thermal stress on equipment
Middle East	Onshore LNG Plant	Equation of State Models	Predicting phase behavior under variability	Enhanced condensate handling and reliability
South America	NGL Fractionation Unit	Dynamic Simulation Tools	Control strategy tuning during shutdowns	Decreased start up times and flaring losses

twin represents a virtual replica of a physical process, dynamically updated with live data. This virtual environment, built using process simulation platforms, enables operators to test various operating scenarios, predict process behavior under upset conditions, and implement corrective measures without disrupting actual operations.

The table below presents a comparative summary of key simulation platforms used in LNG and NGL facilities, highlighting their features, compatibility with real time systems, and industrial applications.

This table provides a detailed comparison of major simulation platforms commonly used in LNG and NGL operations, focusing on their ability to integrate with real time monitoring systems. It outlines the type of simulation each platform supports, their level of compatibility with live data feeds, typical industrial use cases, available data input interfaces, and key strengths in gas processing environments.

Challenges and Limitations

Despite significant advancements in simulation techniques for predicting gas behavior in LNG and NGL operations, several challenges persist that limit their full industrial implementation and predictive reliability. These limitations are often rooted in both technical and operational realities that constrain simulation performance in real-world environments.

One major challenge is the incompleteness of thermodynamic data for complex gas mixtures. In practical LNG and NGL systems, gas compositions vary widely, and accurate property prediction depends heavily on the availability and quality of component-specific data. Inadequate vapor-liquid equilibrium data, particularly for heavier hydrocarbons and trace compounds, can undermine the precision of even the most advanced equations of state.

Another key limitation is the computational demand associated with high-fidelity simulations. While molecular simulations and dynamic models offer increased accuracy, they often require substantial processing power and longer run-times, making them less feasible for time-sensitive operational decision-making. Furthermore, many field applications lack the infrastructure to support real-time deployment of these computationally intensive tools.

The rigidity of model assumptions also poses a limitation. Many simulation platforms rely on assumptions of ideal or pseudo-ideal conditions that do not always hold under extreme pressures and temperatures typical in cryogenic gas systems. This may result in deviation between simulated outputs and actual process conditions, especially in transient or upset scenarios.

Data integration remains another persistent challenge. The effectiveness of predictive simulation is tied to the availability of high-quality, real-time operational data. In many gas facilities, sensor inaccuracies, calibration issues, and poor data resolution can compromise the integrity of model inputs, thereby reducing output reliability.

Additionally, software and licensing constraints can limit accessibility to advanced simulation platforms. High costs associated with industrial-grade simulators and the need for specialized training reduce the adoption of advanced models, particularly in smaller facilities or regions with limited technical infrastructure.

The following table presents a comparative overview of common limitations associated with the leading simulation techniques used in LNG and NGL operations.

This table presents a structured comparison of the primary simulation techniques commonly employed in LNG and NGL operations, highlighting their respective limitations. It categorizes each technique based on key areas including the specific limitation it faces, the level of computational demand required, its suitability for large-

Table 2: Comparative Summary of Simulation Platforms Integrated with Real Time Monitoring in LNG and NGL Operations

<i>Simulation platform</i>	<i>Type of simulation</i>	<i>Real time integration capability</i>	<i>Primary industrial use</i>	<i>Data input interface</i>	<i>Strengths in lng and ngl operations</i>
Aspen HYSYS	Dynamic and Steady State	High	Process simulation and optimization	OPC, Modbus, custom APIs	Accurate thermodynamic modeling and gas separation
OLGA	Dynamic Multiphase Flow	Medium	Flow assurance and transient analysis	OPC, PI System	Excellent for multiphase pipeline modeling
PRO II	Steady State	Low	Plant design and steady process optimization	Manual and limited live feed	Strong for design but limited in dynamic operations
gPROMS	Dynamic and Custom Modeling	High	Custom modeling and parameter estimation	OPC UA, SQL	Highly flexible and useful for research based simulation
Dymola	Multi Domain Modeling	Medium	Physical modeling of complex gas systems	Real Time Toolkits	Useful for integrating mechanical and control models

Table 3: Comparative Overview of Limitations in Gas Behavior Simulation Techniques

<i>Simulation technique</i>	<i>Key limitation</i>	<i>Computational demand</i>	<i>Industrial scalability</i>	<i>Accuracy in complex mixtures</i>
Steady-state process models	Assumes equilibrium conditions	Low	High	Moderate
Dynamic simulation models	Requires real-time data and calibration	High	Moderate	High
Molecular simulation	Intensive computational requirement	Very High	Low	Very High
Equation of State models	Dependent on quality of component data	moderate	High	Moderate to High
CFD-based approaches	High setup complexity and boundary condition needs	High	Low	High

scale industrial application, and its predictive accuracy when dealing with complex gas mixtures.

Future Trends and Research Opportunities

As the LNG and NGL industries continue to expand in scale and complexity, the role of simulation in predicting gas behavior is expected to evolve significantly. Advancements in computational power and modeling frameworks are paving the way for more refined, efficient, and real-time applications in gas processing. Several emerging trends point toward a future where predictive accuracy, operational responsiveness, and model adaptability will be central to industry success.

One of the most significant directions is the gradual integration of data-driven techniques with traditional simulation models. Machine learning and artificial intelligence are being explored as complementary tools capable of enhancing pattern recognition and anomaly detection in gas behavior. These approaches show potential in accelerating the calibration of thermodynamic models and improving forecasting in rapidly changing operational conditions.

Another key development involves the adoption of cloud-based simulation environments. These platforms facilitate remote modeling, collaborative analysis, and dynamic scalability which are particularly valuable for multi-location operations. Cloud simulation environments also support continuous model updates, enabling operators to maintain simulation accuracy across diverse feed compositions and process loads.

Efforts are also underway to develop hybrid modeling frameworks that combine rigorous physical models with empirical datasets. This fusion can result in more robust predictions especially in systems involving non-ideal mixtures or novel process designs. Such hybrid models can adjust to variable field data without compromising theoretical accuracy.

Furthermore, improvements in real-time process monitoring and sensor technologies are enhancing the relevance of simulation-supported decision-making. By embedding simulation feedback into distributed control systems, operators can perform predictive maintenance, fault detection, and process optimization with higher confidence.

Lastly, the evolution of computational fluid dynamics in gas behavior modeling is expected to increase. Although traditionally computationally intensive, recent developments are making CFD more accessible for segment-specific simulation in LNG and NGL pipelines, separators, and heat exchangers. These trends reflect a broader transformation in gas processing where simulation is shifting from a back-end design tool to a front-line operational instrument. Future research should focus on strengthening the interoperability of simulation platforms with control architectures and validating hybrid models under a wider range of gas compositions and environmental conditions.

Conclusion

Gas behavior prediction in LNG and NGL operations has continued to form a very crucial aspect in attaining reliability, efficiency and safety of gas processing operations along the gas processing value chain. The limitations of the old convention based estimation methods are becoming manifested as the composition of natural gases becomes more varied and the processing environments more complex. The paper has demonstrated that more complex simulation methods offer a rigorous and receptive way of modeling the flow and thermodynamic performance of gas mixtures in cryogenic and high pressurized chemical systems.

Appropriate equations of state combined with the dynamic simulation platforms allow operators and engineers to predict system reactions, minimize individual processes conditions and eliminate risks linked with phase changes and hardware limitations. The ability of these simulation tools like Aspen HYSYS OLGA and other process modeling environments to consider multiphase behavior compositional variations and nonlinear process dynamics process modeling environments has made simulation tools to become functional in both design and real-time operations.

But simulation techniques require good quality input data and periodic calibration and trained interpretation to have practical worth. Since the technology of simulation is still in development there is great potential for future development in the integration between simulation

technology and automated control systems concerning process optimization strategies and predictive analytics. The alignment of computer simulation with actual operational data does not only enhance predictive capacity but also enhances better decisions and plant performance.

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