HARNESSING THE POWER OF LNG MODELLING

Nuno Pedrosa, Behnam Salimi, and Shaun Mohammed, KBC (A Yokogawa Company), describe how advanced technology solutions can propel decarbonisation and operational efficiency within the LNG industry.

LNG is not just a fuel choice; it is a key driver in the global energy transition and decarbonisation efforts. This shift from coal and oil to gas as a cleaner fuel source has sparked interest among producers to expand their production capacity through new construction projects and invest in advanced technologies that enhance their current production capabilities.

As a result, the LNG market is witnessing advancements in various technologies. These technologies can add value in many ways, such as:

- Increasing efficiency in asset management.
- Optimising plant staffing levels.
- Accelerating decision making within the supply chain.
- Enhancing Industrial Automation 2 Industrial Autonomy (IA2IA).

SOFTWARE

- Increasing energy efficiency.
- Implementing carbon capture storage solutions.
- Optimising production capacity.

This article will explore why reliable modelling software is crucial to achieve these goals.

Changing LNG landscape

The LNG market is going through dramatic changes, mainly due to two factors: the decarbonisation targets set by numerous countries, and the geopolitical situation which requires many countries to adapt and find new domestic or international sources of LNG.

According to the Global LNG Outlook 2023 – 2027 report from the Institute for Energy Economics and Financial Analysis (IEEFA),[1] a wave of new LNG projects is scheduled from 2025 – 2027. However, the report also signals the potential challenge of weaker-than-expected demand, which could lead to lower prices and profits for LNG suppliers and traders.

On a more positive note, the report also indicates a significant increase in European LNG demand over the past few years. Between 2019 and 2021, Europe relied on imported LNG to meet around 20% of its gas demand. However, in 2022, the proportion of LNG in total gas demand increased significantly, surpassing the 35% mark per the report.

Unlocking maximum benefits

Given these market dynamics, it is even more crucial to have highly optimised processes to maximise the benefits from the existing production capacity. Optimised processes can help LNG producers extract the most value from their operations, improve efficiency, cut costs, and stay competitive in a potentially challenging market.

By implementing advanced technologies, streamlining operations, and enhancing overall productivity, LNG suppliers can position themselves favourably to navigate market uncertainties and leverage the growing European demand.

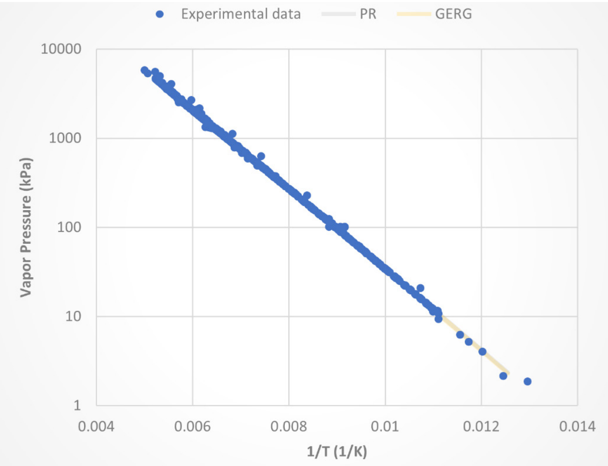

Figure 1. Vapour pressure of methane.

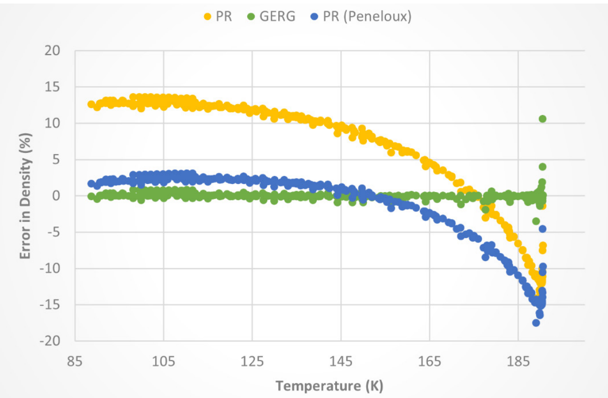

Figure 2. Error in methane predicted density. Peneloux Volume shift was used for the PR model.

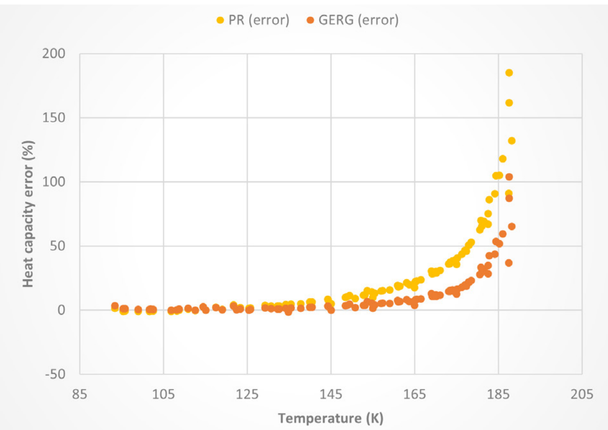

Figure 3. Methane heat capacity at constant pressure error.

Efficient transportation and production

The main purpose of LNG is to have a more efficient way to transport natural gas. It is cheaper to transport liquids than to transport gas, as the transported volume is much smaller for the same amount of gas. Natural gas comes from many kinds of reservoirs, and there are two main types: conventional gas, either from gas fields or gas associated with oil fields, and non-conventional gas, such as tight gas from fracturing, naturally occurring hydrates, and more.

To liquefy natural gas, various commercially-available production packages exist. They are fundamentally based on the same principle: a series of cooling and compressing cycles. The packages primarily differ based on the choice of coolant, number of cycles required, and the inclusion of precooling steps.

Revolutionising process modelling

As described in the previous section, producing LNG, and consequently, its transportation and storage require equipment that can withstand the low temperatures of -161˚C. To minimise CAPEX, it is essential to model fluids and processes accurately and avoid over or under-dimensioning materials.

Traditional process simulation for most of the applications employs cubic equations of state (EoS). These are models that are improvements over the original cubic EoS developed by Van der Waals in the late 19th century,[2] and its principles, with some modifications, are still widely used for general purpose hydrocarbon production and processing.

However, it has important limitations that even the latest modifications have not improved. The main limitation is the low accuracy to predict volume of liquids, and even their compressibility, i.e., how much the volume changes with applied pressure.

LNG process licensors know this, and over the years many have developed their internal multi-parameter models that are maintained by only a few people inside these companies. Operating in this manner carries inherent risks, particularly when the knowledge surrounding these models is lost or inadequately maintained. As time progresses, it becomes increasingly challenging to ensure that the models remain current with the latest developments.

High accuracy equations of state

In recent years, the concerted efforts of many research groups worldwide have been instrumental in reversing this trend. Their work has focused on developing general-purpose models that strive for the highest possible accuracy in predicting key properties that can be measured. These properties typically include volume (density), compressibility, heat capacity, as well as bubble and dew point temperatures and pressures. The main groups dedicated to this initiative are the U.S. National Institute of Standards (NIST) and the European Gas Research Group (GERG). The latter using previous works of various researchers, grouped and improved several EoS known as the GERG-2008 Equation of State (EoS). This EoS is now an ISO standard (ISO 20765-2/3) for natural gas.

The GERG-2008 EoS, while having some limitations in its scope, still shows a satisfactory level of generality when applied to LNG processes. However, challenges arise when dealing with LNG mixtures containing heavier components. In response, a dedicated group of researchers recognised the need for an improved approach and re-parameterised the fundamental equations derived from GERG-2008, specifically tailored to the components of interest in LNG. This re-parameterisation led to the development of a specialised EoS known as EOS-LNG. In this work, the focus was on the following sets of binary mixtures: methane and n-butane, methane and isobutane, methane and n-pentane, and methane and isopentane.

These equations are significantly more complex than the traditional cubic EoS, but with the improvements in computational power, they become usable for these applications and can be used directly in process simulators. The relatively low number of components also helps to make calculations more efficient.

For many years, KBC's Multiflash® technology has included high accuracy models as part of the thermodynamics package, even before GERG-2008 was published. The most current versions have GERG-2008 as well as the purpose-built model for LNG, the EOS-LNG equation. This work shows the improvements in these models compared to each other and in relation to popular versions of cubic EoS: Peng-Robinson (PR). For density predictions with cubic EoS, many attempts have been made to improve it. One of them includes performing a volume shift on the equations as proposed by Peneloux. This version of PR EoS is also considered in the study when comparing density predictions.

Improving LNG models

The performance of three models, namely PR, GERG-2008, and EOS-LNG, have been evaluated for a specific set of components. These models have been assessed based on important properties such as density, Joule-Thomson coefficient, compressibility, heat capacity, and the speed of sound, which is particularly relevant for transportation purposes. Knowledge of these thermophysical properties is very important for precise design and optimising transportation. Although different experimental techniques are available to measure thermophysical properties of fluids, direct measurement at high pressure is difficult for some properties, like the Joule-Thomson coefficient. Therefore, it is preferred to use indirect methods to determine these properties employing other measured properties. The speed of sound in fluids is one of the most useful thermodynamic properties that can be used to determine other thermodynamic properties like density, isobaric heat capacity and Joule-Thompson coefficient. Moreover, in comparison with other thermodynamic properties, the speed of sound can be measured with high accuracy in the laboratory, which makes it very special.

The systems that will be covered are pure methane. After all, LNG is composed mostly of methane, and a simple mixture that covers the typical LNG composition.

However, a preliminary assessment of the models' performance against available experimental data is necessary before proceeding. Methane is the most important component to consider when doing calculations for LNG applications. The plots depicted in Figures 1 through 4 show how the models, PR and GERG, perform when predicting methane properties. For pure components such as methane, GERG, and EOS-LNG perform the same. However, the parametrisation of mixtures distinguishes GERG from EOS-LNG as shown in Figures 5 – 9.

Looking at the results shown in Figures 1 – 4, both models perform relatively well for vapour pressure and heat capacity. The GERG type model is slightly better in predicting heat capacity.

However, the density and speed of sound are not very well predicted. This is a known limitation of the cubic EoS models. They still fall short from experimental data, even when using extra terms to improve density predictions. As seen in Figure 2, it is impossible to get an error below 15%, on average.

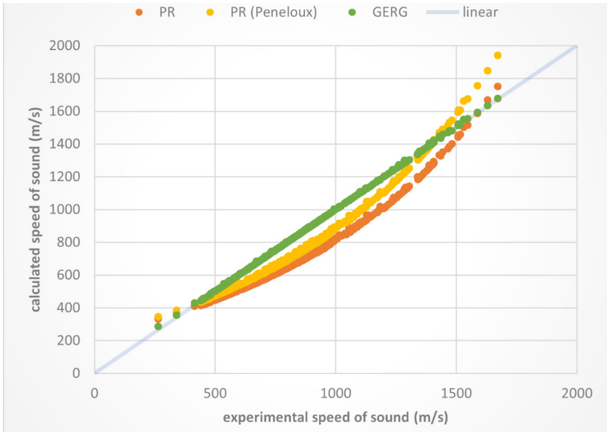

Figure 4. Liquid methane speed of sound.

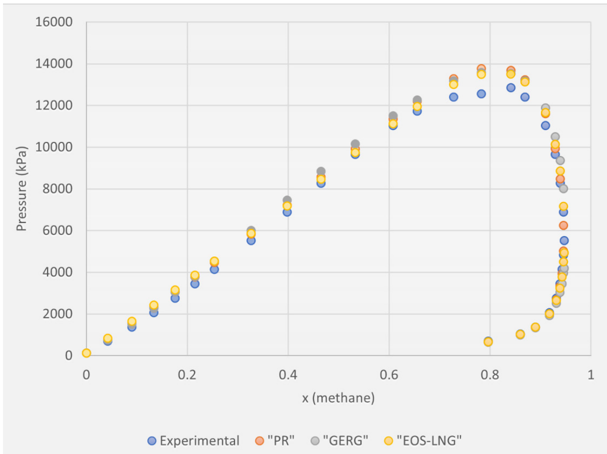

Figure 5. Vapour liquid equilibria between methane and butane.

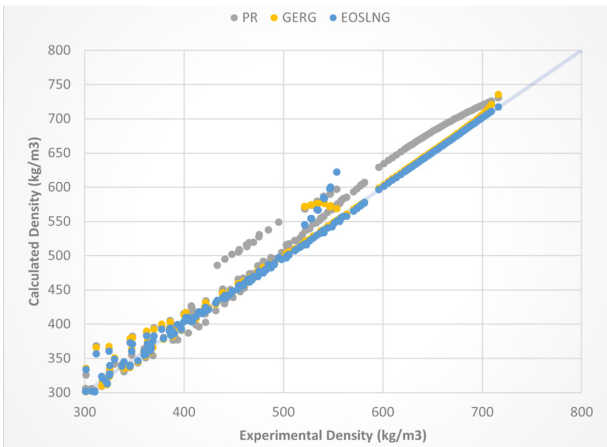

Figure 6. Comparison of density for the system methane/butane

For the system methane/butane, as far as vapour equilibria is concerned, all models perform quite well, as shown in Figure 5. For density, the cubic EoS models show the same limitation as in the pure component case. In Figure 6, they are shown to be much less accurate than GERG or EOS-LNG. As demonstrated in Figure 7, for heat capacity of the methane/butane mixture, EOS-LNG model shows better agreement with experimental data compared to the other models.

Another example where EOS-LNG shows a big improvement to LNG processes is the methane/pentane mixture. As shown in Figure 8, at higher temperatures, EOS-LNG can reproduce the data better than GERG. Interestingly, PR performs quite well, but as Figure 9 depicts, the density predictions by PR are worse than GERG or EOS-LNG models, particularly for higher densities, where LNG is of interest.

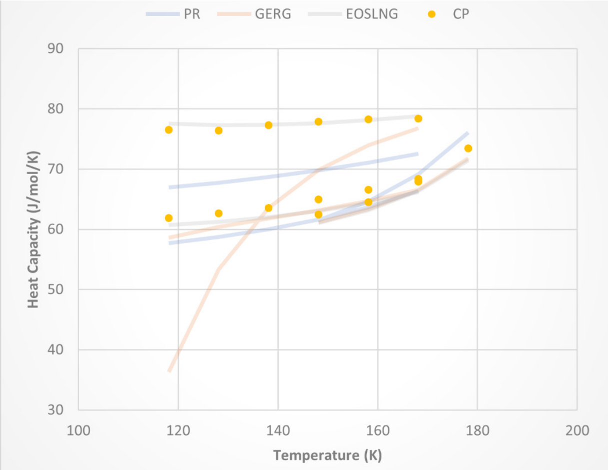

Figure 7. Heat capacity at constant pressure for the system methane/butane.

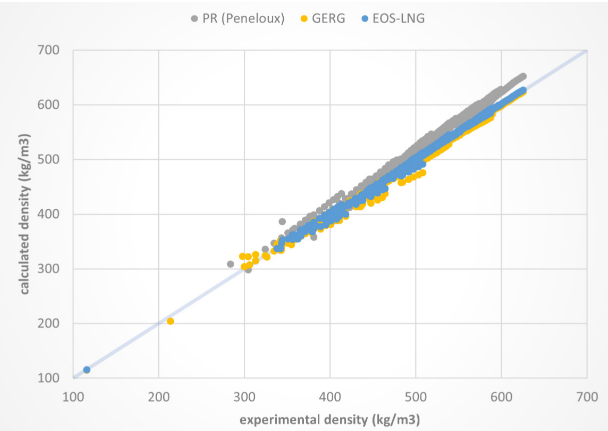

Figure 8. Liquid density for methane/pentane mixtures. Comparison with experimental data.

Conclusion

Processing natural gas for LNG has been a long-standing practice, but the accuracy and applicability of models have historically lagged. However, thanks to the rapid advancements in computer technology, more precise models can be made readily available to a broader audience. By incorporating these advanced models into the process-solving approach, the reliability of the results can be significantly improved.

Integrating accurate models into process simulation enhances equipment sizing to perfectly match the requirements without unnecessary oversizing or undersizing. This optimisation can lead to cost savings, increased efficiency, and improved overall performance.

Moreover, reliable models aid in assessing the correct values of utilities employed in the process. By accurately estimating the required utilities, such as energy inputs or cooling water, operators can optimise resource utilisation and enhance the overall sustainability of LNG production while minimising waste.

With wider accessibility of more accurate models, users can make informed decisions based on reliable predictions. This not only improves the overall operational efficiency but also reduces uncertainties and risks associated with process design and optimisation.

In summary, advanced modelling tools enable more accurate predictions and wider applicability in LNG processing. By leveraging these models, operators can ensure proper equipment sizing, optimise resource utilisation, and make informed decisions to enhance the reliability and efficiency of the LNG production process. **LNG**

References

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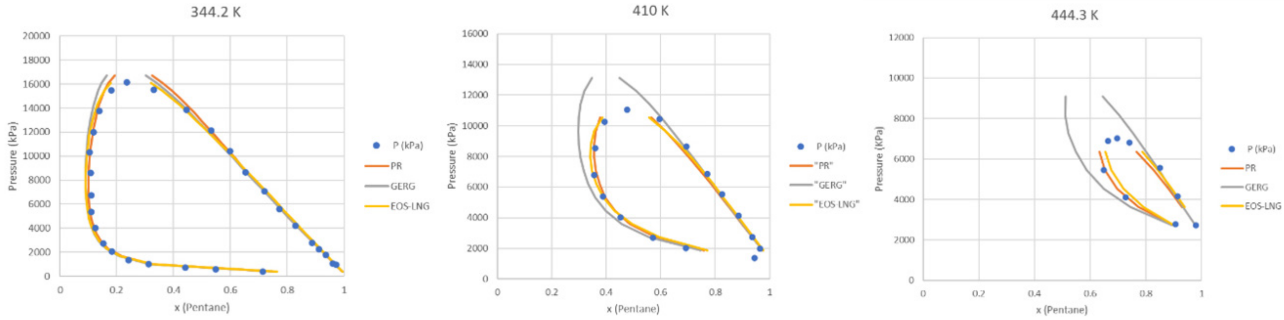

Figure 9. Vapour-liquid equilibria for methane-pentane (data from Sage et 1942).