HYDROGEN'S PURE POTENTIAL

Garry Hanmer, Senior Simulation Consultant, Atmos International, UK, evaluates how to accurately model pure hydrogen pipelines, using a case study to demonstrate the model tuning process and the selection of appropriate equations of state.

The need for a shift in energy generation, transportation and usage to fulfil climate change objectives is acknowledged worldwide, with parties at COP28 agreeing to accelerate decarbonisation efforts.[1] While several competing technologies are vying for a role in this energy transformation, this article concentrates on the potential of hydrogen. Hydrogen provides an opportunity to leverage the existing extensive infrastructure of the fossil fuel industry and hydrogen blends, but there are risks involved.

High pressure steel transmission pipelines face a significant threat from hydrogen embrittlement, which can lead to cracking, blistering and weakness. This occurs when hydrogen infiltrates the pipeline material, causing corrosion of the steel pipe, valves, and fittings.

Using a case study that examines the implementation of a real-time system for simulating hydrogen pipelines, this article will evaluate the precision of various equations of state by utilising an operational pure hydrogen pipeline.

Hydrogen transportation

Transporting hydrogen in large commercial quantities is challenging due to its unique properties. The smaller size of the hydrogen molecules compared to natural gas allows it to diffuse with the pipeline material, leading to hydrogen embrittlement and the deterioration of the steel pipes.

Hydrogen also has a lower energy density than natural gas, requiring larger diameter pipelines to transport the same amount of energy. This makes long-distance transportation more expensive and less efficient.

While repurposing natural gas pipelines for hydrogen transportation can be beneficial it does require an analysis of operating procedures. Pipeline simulation can assist by modelling the changes in pipeline capacity with the change in fluid.

Figure 1. Differences between calculated and measured pressure over 27 days.

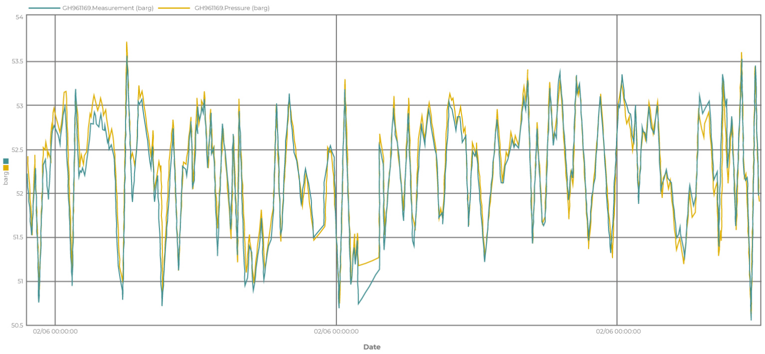

Figure 2. Measured pressure (in green) versus calculated pressure (in yellow) over 27 days.

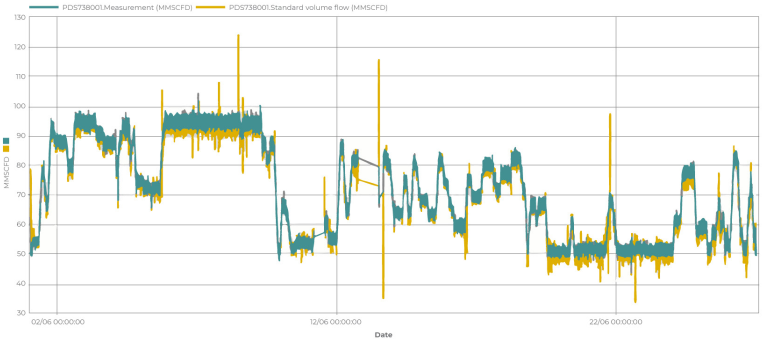

Figure 3. Measured flow (in green) versus calculated flow (in yellow) over 27 days.

Hydrogen embrittlement risks

Hydrogen embrittlement is a process that occurs when hydrogen atoms are absorbed into a metal, causing it to become brittle and susceptible to cracking and fracture. This occurs when hydrogen atoms diffuse into the metal lattice, causing lattice distortion and weakening the metal's ability to withstand stress.

Hydrogen embrittlement can occur in a variety of ways, but in the pipeline industry it's commonly associated with when metals are exposed to hydrogen gas or other hydrogen-containing compounds, such as water vapour or hydrogen sulfide.

Preventing hydrogen embrittlement requires a combination of measures, including proper material selection, design and maintenance. In many cases, it's essential to use materials that are resistant to hydrogen embrittlement, such as high-strength alloys, that have been specifically designed to resist hydrogen embrittlement.

Ensuring the safety of the public in industries such as hydrogen energy, chemical and oil refineries requires careful consideration of hydrogen embrittlement. The selection of a suitable pipeline material is critical in reducing the risk of this phenomenon. An alternative approach to reducing the risk of hydrogen embrittlement is the reduction of the concentration of hydrogen. This can be achieved by blending hydrogen with compounds such as natural gas to dilute the concentration.

The following case study demonstrates how an accurate hydrogen model can be achieved by the model tuning process and the selection of appropriate equations of state so that it can provide a more accurate prediction of the pipeline areas subject to hydrogen embrittlement.

Case study: pure hydrogen pipeline

Spanning 160 km from west to east, this pipeline has a mainline section divided into two branches with the southernmost branch splitting into two parallel pipes.

Model tuning process

To achieve the required accuracy and reliability of the online model, it is essential to tune the configuration parameters to match actual operational data from the physical pipeline. Operational data was collected for a 27 day

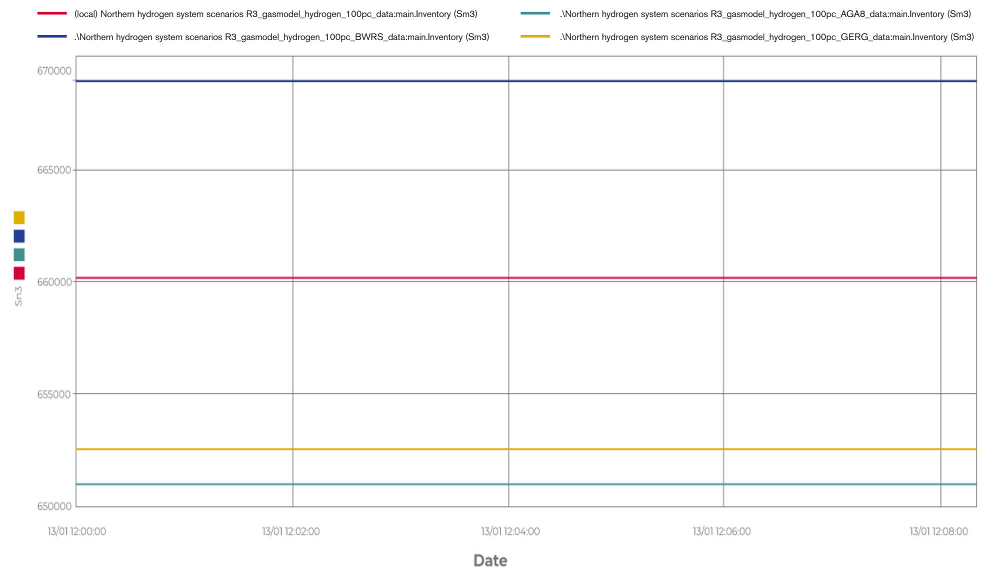

Figure 4. EOS comparisons for pure hydrogen.

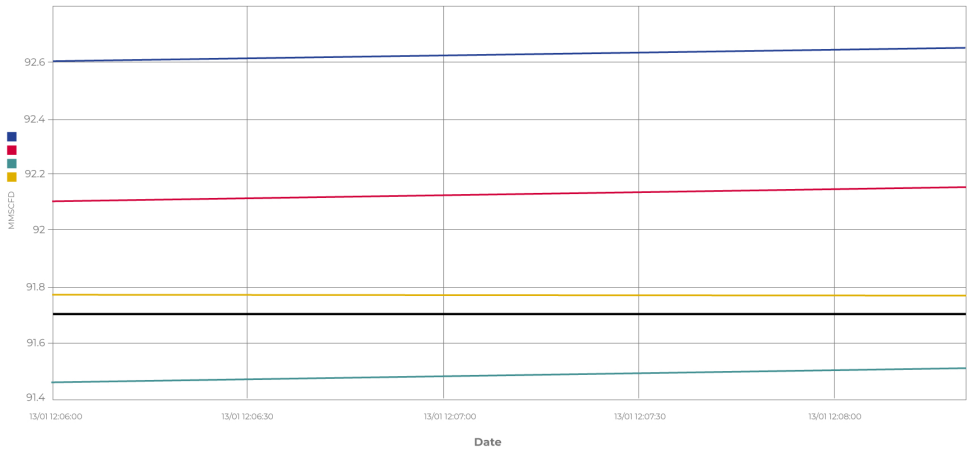

Figure 5. EOS flow comparisons for pure hydrogen.

period and a shorter dataset was extracted for seasonal comparison purposes. By minimising deviations between the model's calculated values and the physical pipeline's data, the model can be tuned.

The aim of the tuning exercise is to ensure the network line pack, pressure, flow and temperature calculations are accurate. To achieve this, the pipeline roughness property is adjusted for tuning the network line pack and the heat transfer property is tuned for the temperature profile. By adjusting these two properties, an accurate pipeline pressure drop for a specific flowrate can be achieved.

A controlled reference case is selected from the datasets for tuning the pipeline roughness and heat transfer properties. This reference case involves analysing stable periods where the flowrates are at or near the pipeline's capacity flowrates. It is then imported into an offline simulation for tuning purposes.

The tuning of the network line pack and pipeline temperature profile directly affect each other so an iterative approach is necessary for tuning these properties. By tuning these properties, an alignment can be achieved between the physical pipeline and the simulated pipeline for network line pack and flow, pressure and temperature.

The process for tuning of the temperature profile should follow the tuning of the pipeline capacity, forming the following steps:[2]

1. Offline roughness tuning to the controlled reference case.
2. Online analysis of the temperature metre deviations between measurement and calculated values.
3. Offline heat transfer tuning.
    a. Tune the soil conductivity of buried and partly buried sections to achieve an accurate temperature profile.
4. Offline roughness tuning re-adjust (point 1).
5. Deploy tuned configuration online.
6. Online analysis of the temperature metre deviations (point 2).
    a. Repeat the above steps until the target discrepancy in the temperature profile is achieved.

After the initial tuning is completed, a second sample period is used to validate the tuning. The simulation is run against the entire sample period to confirm the accuracy of the model. The differences between the calculated and measured pressure over the 27 day sample period can be observed (Figure 1).

Figure 1 illustrates the difference between all the calculated and measured pressure from the network and a high level of consistency with an error of less than 0.2 bar throughout the sample period, equivalent to over 99.7% accuracy.

Looking closer at the accuracy of the modelled pressures, we can examine the measured and calculated values of a particular pressure metre. Figure 2 displays the measured pressure (in green) and calculated pressure (in yellow) for the 27 day sample period, demonstrating the automatic tuning of the online model.

The precision of the calculated flows can also be evaluated by examining the measured and calculated values of one of the pipeline flowmeters. Figure 3 illustrates the measured flow (in green) and calculated flow (in yellow) during the 27 day sampling period.

The most appropriate equation of state for modelling pure hydrogen

A suitable equation of state (EOS) for the modelling of pure hydrogen is required to be applicable for compositional fluids and to be accurate for the operational range of pressures and temperatures observed within the extracted data. While there are other considerations for the choice of equation (ie. performance and accuracy) these would be evaluated as part of the analysis.

The below equations of state were chosen for this case study.

GERG

The GERG EOS is a cubic equation that relies on the composition of gas mixtures and a thermodynamic model to describe their properties. It's based on the principle of corresponding states, which suggests that gases with similar reduced properties exhibit similar thermodynamic properties. This equation is particularly useful for modelling natural gas mixtures but can also be used for hydrogen blends.

Numerous validations have confirmed GERG's ability to accurately predict the thermodynamic properties of natural gas mixtures. When applied to hydrogen blends, this equation can forecast properties like density, viscosity, and compressibility factor. However, it assumes that the gases in the mixture do not interact, which may result in inaccuracies in the predicted thermodynamic properties.

AGA8

AGA8 is a cubic EOS that uses composition-based methodology to determine the thermodynamic characteristics of natural gas and gas blends. This equation of state has undergone extensive verification and is grounded in empirical data. AGA8 is based on a broad set of experimental data on natural gas and gas blends, which is frequently updated to ensure that it remains precise and relevant. However, AGA8 assumes ideal gas behaviour, which may not be valid for hydrogen blends under certain circumstances. At high pressures and low temperatures, hydrogen's behaviour can diverge from ideal gas behaviour, resulting in inaccuracies in simulation outcomes.

Peng Robinson

Peng Robinson is a thermodynamic model that utilises a composition-based cubic EOS to calculate fluid properties. It follows the theory of corresponding states, which asserts that fluids at the same reduced temperature and pressure display similar characteristics. This equation is commonly used in the oil and gas industry to simulate the behaviour of natural gas and hydrogen blends. The Peng Robinson EOS has been extensively tested and validated across a broad spectrum of fluids and is simpler than other equations of state while still being capable of modelling mixtures with intricate compositions.

A limitation of using Peng Robinson to simulate hydrogen blends is its failure to account for any chemical reactions that might occur in the blend. Such reactions, such as the interaction between hydrogen and other gases in the blend, can alter the properties of the mixture.

Benedict Webb Rubin Starling (BWRS)

BWRS employs a non-cubic composition-based approach to relate a fluid's pressure, temperature, and volume to its molecular properties, using a thermodynamic model. While typically used for modelling hydrocarbon mixtures such as natural gas, it is also applicable to hydrogen blends. This equation is rooted in statistical mechanics.

BWRS can predict the thermodynamic properties of hydrogen blends and provides an accurate understanding of the behaviour of the fluid as it moves through the pipeline, as well as for designing pipeline systems that can handle different concentrations of hydrogen.

Equations of state in the context of a real pure hydrogen pipeline

The pipeline capacities for the case study pipeline using pure hydrogen are displayed in Figure 4. The GERG 2004 capacity is shown in orange, BWRS in blue, AGA8 in green and Peng Robinson capacity in red.

We can evaluate the EOS by comparing their flowrate calculations with the measurements obtained from the dataset.

Figure 5 illustrates these comparisons, where the flowrates obtained from the GERG 2004 equation are depicted in orange, BWRS in blue, AGA8 in green, Peng Robinson in red, and the actual measured flowrate in black.

Compared to the measured values, the Peng Robinson EOS exhibited an error of 0.97%, while the AGA 8 and BWRS equations of state exhibited deviations of 0.27% and 0.43% respectively. In contrast, the GERG 2004 equation of state exhibited deviations of only 0.05%.

To conduct this analysis, an offline simulation was performed for each equation of state, with pressure set as the boundary conditions. These pressure setpoints were a part of the controlled reference case that was discussed in the model tuning section above. The simulation then calculated the flowrates for each equation of state, which were subsequently compared against the measured flows observed in the controlled reference case.

The undeniable importance of hydrogen modelling

Hydrogen plays a crucial role in the future of global energy and the increasing demand for renewable energy sources requires pipelines to be an integral part of the infrastructure. Accurately modelling hydrogen pipelines is essential to mitigating as much risk as possible.

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