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How Gas Pipeline Operating Imbalances can be Improved with detailed Line Pack Calculations?

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1 INTRODUCTION

In the realm of natural gas transportation, pipeline networks are indispensable as they offer a reliable and cost-effective means of distributing natural gas from production sites to end-users. Maintaining the integrity and balance of gas pipelines is crucial to ensure a consistent supply while minimizing disruptions and environmental impacts.

A gas pipeline comprises pipe segments and assorted equipment. To assess pipeline integrity and the performance of metering systems, a balance over the pipeline can be calculated. EU Commission Regulation No 312/2014 mandates the daily imbalance calculation, and daily imbalance charges may apply. An imbalance exceeding permissible limits may indicate issues with metering systems, line pack calculations, or the presence of leaks or losses, and may result in financial consequences.

As well as the accuracy of the pipeline inlet and outlet metering systems, line pack calculations are key elements in gas pipeline imbalance calculations and should be carefully developed or selected. Multiple off-the-shelf tools are available along with tools developed in-house.

This paper addresses questions about selecting the most reliable/trustworthy tools for line pack calculation, considerations during configuration, the importance of validation, and which values to trust when multiple tools are in use. Additionally, it covers the specifics of CO₂ and H₂ from the perspective of line pack calculations.

Section 2 covers the concept of pipeline imbalance and establishes the limits for imbalance based on operational and financial constraints. It demonstrates the importance of accurate line pack calculation and highlights differences in results across various applications, thereby introducing the challenge of selecting the most accurate one.

Section 3 delves into line pack calculation methods, differentiating between simplified and detailed methods. It describes offline and online applications, with a particular focus on the latter by comparing Pipeline Application System (PAS) and Leak Detection System (LDS) pipeline simulators. The comparison of calculation results for all applications is provided, and a conclusion on the most accurate calculation method is presented. The section also discusses the necessity of configuration and calculation validation, along with the advantages and disadvantages of applications developed in-house or purchased from a provider.

Section 4 examines the specifics of pipeline simulators associated with other fluids, namely CO₂ and H₂, transported through pipeline. Section 5 presents the conclusions. Section 6 contains the abbreviations.

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2 PIPELINE INTEGRITY AND IMBALANCE

In the context of pipeline integrity, it is crucial to ensure that the balance in terms of standard volume (mass or energy) within a pipeline is maintained.

2.1 Imbalance Equation

Physically, an imbalance occurs when the amount of gas delivered into the pipeline during a specific time period (for example, one gas day) does not match the sum of the gas off-taken, vented or unaccounted for during pipeline operation, the gas taken from the pipeline, and any changes in line pack when a line pack flexibility service is provided within the same period of time.

EU Commission Regulation (EU) No 312/2014 [1] in article 21 mandates that the transmission system operator (applicable to other pipeline operators) is responsible for computing an imbalance on each gas day, as per the formula outlined below:

$$Im_d = In_d - [Out_d + FG_d + Vent_d + (LP_d - LP_{d-1})] \quad (1)$$

Where:

- Im_d is the physical imbalance on gas day 'd', Sm^3 . This imbalance is reflected in storage terms and should be limited by the line pack flexibility and the uncertainty of the measured and calculated variables.
- In_d is the total gas injected into a pipeline and measured by a metering system at the pipeline Entry Point on gas day 'd', Sm^3
- Out_d is the total gas taken from a pipeline and measured by a metering system at the pipeline Exit Point on gas day 'd', Sm^3
- FG_d is the total fuel gas used on gas day 'd', Sm^3 . The gas is used as fuel in compressors, which provide the energy necessary to operate a pipeline.
- $Vent_d$ is the total vented gas on gas day 'd', Sm^3 . The gas is intentionally released for operational or safety reasons during pipeline operation.
- LP_d is the line pack calculated at the end of gas day 'd', Sm^3
- LP_{d-1} is the line pack calculated at the beginning of gas day 'd' what is the same as the line pack at the end of the previous gas day 'd-1', Sm^3 .

The gas unaccounted for (losses mainly caused by measurement errors, data quality issues, leaks and fugitive emissions) can be added into Equation (1) if it is quantifiable. However, in the context of this paper, it is not taken into consideration.

In some pipelines, line pack is not considered at all, which is acceptable for incompressible or nearly incompressible fluids. However, for compressible fluids, line pack will influence the imbalance and should be taken into account in the imbalance equation.

Where the inputs on the gas day are equal to the sum of off-takes, a pipeline is deemed balanced for that gas day. Otherwise, the pipeline is deemed imbalanced and daily imbalance charges may be applied.

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The daily imbalance charges are calculated in line with a methodology approved by a national regulatory authority or by the interested parties. Usually, to calculate the charges, the pipeline operator shall multiply a daily imbalance quantity by an applicable price. The charges may apply to the whole daily imbalance, or only to its part exceeding the permissible limits.

The presence of imbalance exceeding the predefined permissible limits can serve as an indicator of potential issues with metering systems, the calculation of pipeline line pack, or operating faults such as leaks, valve malfunctions, pressure irregularities, etc. When such imbalances occur, additional investigation is warranted to maintain the integrity and performance of the pipeline system.

2.2 Permissible Limits for Imbalance

The permissible limits should be defined based on the line pack flexibility (operational limit) and the uncertainty of the measured and calculated variables (financial limit) as defined in Equation (1). If the limits are not set correctly, the charges may be applied daily or not at all.

2.2.1 Operational Limit

The operational limit for imbalance is defined by the line pack flexibility. It's important to distinguish between two terms: "Line Pack" and "Line Pack Flexibility".

Line Pack refers to the total volume of gas in a pipeline at any given time. It depends on factors such as pressure, temperature, pipeline volume, and gas composition. All these factors vary locally, posing challenges for a line pack calculation, particularly in long pipelines with changes in elevation and operating conditions.

Various methods, such as SLP, LDS, and PAS (as discussed in Section 3), can be used to calculate line pack. The primary goal is to ensure that the difference in line pack between the beginning and end of a gas day 'd', as expressed in equation (1), remains within the limits defined by line pack flexibility.

Line Pack Flexibility serves as a buffer that arises due to technical constraints, dictating the maximum allowable change in line pack over the gas day [6]. This change can occur by adjusting operating pressure in response to transportation demand profiles. Line pack flexibility is determined by operational requirements and constrained by normal operating range limits.

For example, in pipelines with steady operations, line pack flexibility can be defined as 0.1 % of the pipeline's capacity, allowing it to accommodate daily ambient temperature and operating conditions variations.

2.2.2 Financial Limit

The pipeline imbalance is evaluated based on the daily measured and calculated variables as shown in Equation (1). All variables are identified as the pipeline inlets and outlets and have attributed to them uncertainties. These uncertainties

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are determined either by the metering systems if measured directly or by calculation methods if measured indirectly or assessed mathematically.

The uncertainty of the pipeline imbalance defines the fiscal limits within the imbalance can be justifiably observed. The imbalance uncertainty is calculated by combining the uncertainties of all identified inlet and outlet measured variables [2]. The absolute expanded uncertainty of the pipeline imbalance can be calculated as:

$$u_{Im_d} = \sqrt{\left(\text{In}_d \cdot \frac{U_{In_d}}{100\%}\right)^2 + \left(-\text{Out}_d \cdot \frac{U_{Out_d}}{100\%}\right)^2 + \left(-\text{FG}_d \cdot \frac{U_{FG_d}}{100\%}\right)^2 + \left(-\text{Vent}_d \cdot \frac{U_{Vent_d}}{100\%}\right)^2 + \left(-\text{LP}_d \cdot \frac{U_{LP_d}}{100\%}\right)^2 + \left(\text{LP}_{d-1} \cdot \frac{U_{LP_{d-1}}}{100\%}\right)^2 - 2 \cdot r(\text{LP}_d, \text{LP}_{d-1}) \cdot \left(\text{LP}_d \cdot \frac{U_{LP_d}}{100\%}\right) \cdot \left(\text{LP}_{d-1} \cdot \frac{U_{LP_{d-1}}}{100\%}\right)} \quad (2)$$

Where:

- u_{Im_d} is the absolute expanded uncertainty of pipeline daily imbalance, Sm^3
- U_{In_d} is the relative expanded uncertainty of the pipeline inlet fiscal metering systems, %. The uncertainty of 1 % is considered for the dry gas fiscal applications.
- U_{Out_d} is the relative expanded uncertainty of the pipeline outlet fiscal metering systems, %. The uncertainty of 1 % is considered for the dry gas fiscal applications.
- U_{FG_d} is the relative expanded uncertainty of the fuel gas metering systems or assessed values, %. The uncertainty of 1 % is considered for the measured values.
- U_{Vent_d} is the relative expanded uncertainty of the vented gas measured or assessed values, %. The uncertainty of 10 % is considered for the assessed values.
- U_{LP_d} is the relative expanded uncertainty of line pack at the end of the gas day, %. The uncertainty of 0.15 % is considered for the assessed value (refer to Section 3.1).
- $U_{LP_{d-1}}$ is the relative expanded uncertainty of line pack at the beginning of the gas day, %. The uncertainty of 0.15 % is considered for the assessed value (refer to section 3.1).
- $r(\text{LP}_d, \text{LP}_{d-1})$ is the correlation coefficient between the line pack at the beginning and at the end of the gas day, dimensionless. The correlation coefficient is considered only for the line pack since the same set of measurement instruments and calculation methods apply to both line pack values at the beginning and end of a gas day 'd' in Equation (2).

In the context of this paper, field data of the operating pipeline is considered for imbalance calculation and uncertainty calculation. The pipeline comprises one inlet, one outlet, fuel gas offtakes, and vents.

The calculation results of pipeline imbalance and its associated uncertainty for the representative daily totals are provided in Table 1. The correlation coefficient has been determined to be unity, and it is noteworthy that the imbalance uncertainty remains unaffected by the line pack and solely dependent on the uncertainty of the metering systems at the Entry and Exit points. The sensitivity coefficients are established by algebraic or differentiation as per the principles given in GUM [2].

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At the uncertainty requirements defined above, the imbalance uncertainty is determined to be 77.326 kSm³, which represents approximately 1.5 % of the daily throughput or 0.06 % of the pipeline line pack. Consequently, it is recommended that permissible limits for imbalance should not be set lower than the calculated imbalance uncertainty. If the established limits are higher than expected, efforts should be made to reduce the uncertainty associated with the measured variables.

Table 1 – Daily Imbalance Uncertainty

Title	Value	Sensitivity Coefficient	Expanded Uncertainty	
			Relative, %	Absolute, kSm ³
Entry Point (measured), kSm ³	5,524.648	1.00	1.00	55.246
Exit Point (measured), kSm ³	5,409.843	-1.00	1.00	54.098
Fuel Gas (measured), kSm ³	22.629	-1.00	1.00	0.226
Vent (calculated), kSm ³	7.566	-1.00	10.00	0.756
Line Pack 'd' (LDS calculated), kSm ³	130,399.545	-1.00	0.15	195.599
Line Pack 'd-1' (LDS calculated), kSm ³	130,352.051	1.00	0.15	195.528
Line Pack Correlation Coefficient, dimensionless	1.00	-2.00	-	76,490.317
Daily Imbalance, kSm³	37.116	-	-	77.326

2.3 Imbalance Calculation Results

To calculate the imbalance, one must have both the measured and calculated inputs of the variables defined in Equation (1). The real field data is employed within this article for demonstration purposes.

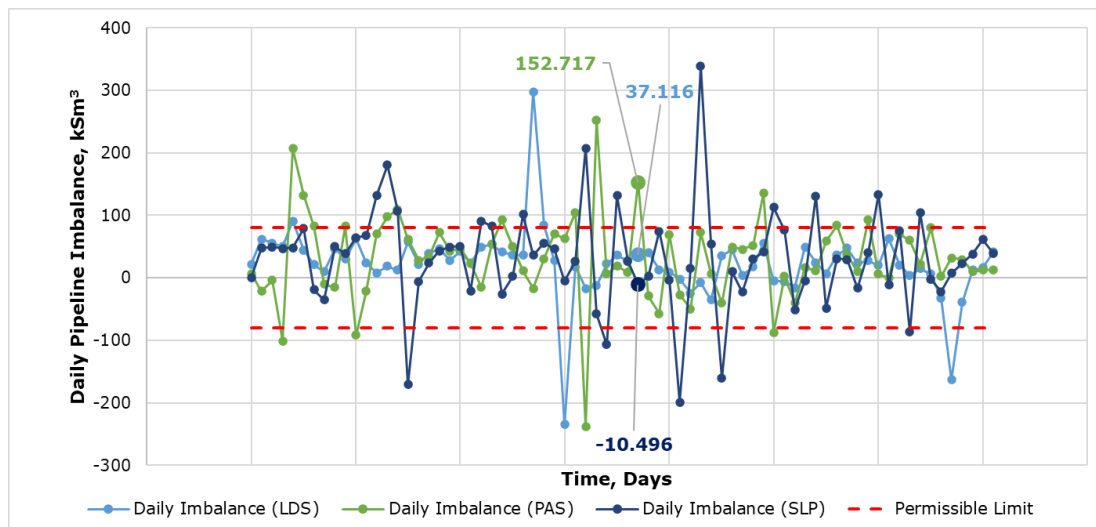


Figure 1 – Pipeline Imbalance using LDS, PAS, SLP

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The results of the imbalance calculation for the pipeline over a three-month period are depicted in Figure 1. The imbalance is computed using the same Equation (1), but the pipeline line pack calculation methods differ. Three methods are considered for the line pack calculation (SLP, PAS, LDS), and they are explained in Section 3.

The calculated imbalance is compared with the limits denoted by the red dashed lines in these figures. These permissible limits are defined by the imbalance uncertainty calculated in Section 2.2.2. Only one out of three methods allow keeping the calculated imbalance predominantly within the limits (LDS) and may be considered as more consistent and reliable.

There are clear differences between the obtained results. To quantify these differences, a single day from the three-month period has been selected, which is depicted by the bigger-sized marker on the figures. The necessary data for the imbalance calculation over this day is provided in Table 2.

Three different pipeline imbalances are obtained, creating a lack of clarity regarding which value to use for reporting. The choice of method might have consequences, including the potential for financial charges if the permissible limits for imbalance are exceeded.

The difference in the calculated imbalances is driven by the line pack calculation method. Therefore, there is a clear need for an investigation to ascertain which calculation method is the most accurate in order to mitigate potential financial charges and ensure the proper pipeline operation.

Table 2 – Line Pack Calculation Results

Parameter, kSm ³	Symbol	LP Calculation Method		
		SLP	PAS	LDS
Entry Point	In_d	5,524.648		
Exit Point	Out_d	5,409.843		
Fuel Gas	FG_d	22.629		
Vent	$Vent_d$	7.566		
Line Pack 'd'	LP_d	130,117.699	130,849.429	130,399.545
Line Pack 'd-1'	LP_{d-1}	130,022.593	130,917.536	130,352.051
Line Pack Difference	$LP_d - LP_{d-1}$	95.106	-68.107	47.493
Daily Imbalance	Im_d	-10.496	152.717	37.116
Permissible Limits	u_{Im_d}	77.326		

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3 LINE PACK CALCULATION

There are multiple line pack calculation methods. However, within this article, only three are compared due to availability of field data.

The first method is the simplified calculation of line pack (SLP). Usually, this calculation is developed during the design stage and based on pipe geometry and operation conditions required for the volume calculation at reference conditions.

The other two are the detailed calculation of line pack, which are off-the-shelf software applications: Pipeline Application System (PAS), designed for decision support; and Leak Detection System (LDS), designed for accurate and robust leak detection.

3.1 Simplified Line Pack Calculation

The simplified line pack calculation (SLP) is usually designed for estimation of gas required to pack the pipeline and at a later stage may be commissioned into daily operation to monitor the pipeline imbalance.

The ideal gas law equation compensated for compressibility is usually deployed requiring the gas temperature, pressure and composition for calculation of compressibility which accounts for the deviation of real gases from ideal behaviour, as follows:

$$LP = \sum_{i=1}^N V_i \cdot \frac{Z_{0i}}{Z_i} \cdot \frac{P_i}{P_0} \cdot \frac{T_0}{273.15 + T_i} \quad (3)$$

Where:

LP	is the pipeline line pack at reference conditions, Sm ³
V	is the volume of pipeline leg at operating conditions, m ³ . The volume is calculated using the internal pipe diameter and its length.
Z ₀	is the compressibility at reference conditions 15 °C (or 20 °C, 60 °F, 0 °C) and 1.01325 bara, dimensionless
Z	is the gas compressibility at operating conditions, dimensionless
P	is the gas pressure measured by pressure transmitters upstream of a block valve and corrected to pipe elevation, bara
P ₀	is the reference pressure of 1.01325 bara
T ₀	is the reference temperature, K.
T	is the gas temperature measured by temperature transmitters upstream of a block valve, °C
N	is the number of pipeline legs.

The uncertainty of a line pack volume at reference conditions stored in a single pipeline leg combines the uncertainties of the input variables listed in Equation (3). The following values can be meaningfully assigned to the variables for the uncertainty calculation:

- Internal pipe diameter uncertainty, 5 mm
- Leg length uncertainty, 50 m
- Reference compressibility uncertainty, 0.1 %
- Gas compressibility uncertainty, 0.1 %

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- Gas temperature uncertainty, 0.5 °C
- Gas pressure uncertainty, 0.2 barg
- Atmospheric pressure uncertainty, 10 %

The uncertainty calculation result for a single pipeline leg is provided in Table 3 for indicative purpose only. The main contributors to the uncertainty are gas pressure and internal pipe diameter. The relative expanded uncertainty of a single leg is calculated as **0.86 %**. Combining the uncertainties of all pipeline legs (for example, 33 legs), the overall uncertainty will be calculated as **0.15 %** considering that the uncertainties of the pipe legs are uncorrelated. The more legs the pipeline consist of, the lower the uncertainty of the line pack will be.

Table 3 – Line Pack Leg Uncertainty

Title	Input Quantity	Relative Expanded Uncertainty %	Divisor	Relative Standard Uncertainty %	Sensitivity Coefficient	
Internal Pipe Diameter, m	1.40	0.357	2.00	0.179	2.000	0.357
Leg Length, m	41,000	0.122	2.00	0.061	1.000	0.061
Reference Compressibility	0.9977	0.100	2.00	0.050	-1.000	-0.050
Gas Compressibility	0.8651	0.100	2.00	0.050	1.000	0.050
Gas Pressure, barg	52.00	0.385	2.00	0.192	0.985	0.189
Atmospheric Pressure, bara	0.79	10.000	2.00	5.000	0.015	0.075
Gas Temperature, °C	5.40	9.259	2.00	4.630	-0.019	-0.090
Leg Volume, kSm³	3,923.077	0.86	2.00	0.43	-	-

The line pack calculations presented in this section are simplistic, and their simplicity is accompanied by limitations. Typically, they are lacking access to real-time data and omitting considerations of radial heat transfer and friction due to pipeline roughness.

Furthermore, the use of more complex equations of state, which account for the specific properties of the gas mixture, may be necessary to accurately calculate compressibility. Consequently, this line pack calculation might become quite complex, especially when a pipeline consists of multiple legs with varying pressures, temperatures, and gas compositions.

It is important to note that these simplified calculations are effectively time-independent in nature and cannot determine whether the line is packing or unpacking, or at what rate the change is occurring, all of which are crucial for pipeline operation.

While these basic calculations serve as a fundamental tool for estimating gas requirements in pipeline operation, it is recommended to incorporate real-time models that encompass the full set of equations of state and can significantly

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enhance the precision and responsiveness of pipeline operations. Therefore, it is advisable to consider the use of off-the-shelf software tools or specialized engineering software that employs a detailed line pack calculation.

3.2 Detailed Line Pack Calculation

Off-the-shelf software applications, such as pipeline simulators, for line pack calculation also come with their own set of advantages and disadvantages. Before delving into a detailed analysis, let's review the types of packages available on the market.

In general, a pipeline simulator serves as a digital twin of the pipeline. It includes a comprehensive mathematical model of the transient flow of fluids through pipeline itself as well as through the associated pipeline equipment. Utilising the pipeline operating data, which typically includes pressures, temperatures, flows, and gas composition usually available at the pipeline inlet and outlet, enables estimates of the operating parameters at all points throughout the pipeline.

3.2.1 Offline Desktop Applications

There are pipeline simulators that are used as a desktop CAE (Computer-Aided Engineering) tool. The fundamental principles underpinning the simulator are the same as detailed above but the method of operating data input is entirely manual. Such simulators are often referred to as "offline" simulators. An example of such a simulator is PipelineStudio (PLS).

Offline pipeline simulators allow the user to quickly and easily configure a pipeline system, including inline equipment such as valves, regulators and compressors. Steady-state or transient analyses can be undertaken to provide insight into the behaviour of the pipeline system under many and varied conditions. Engineers can perform flow assurance studies, design and size pipelines, analyse upsets, surges and leaks, plus many other types of analyses and studies. Such tools can be used to provide the required line pack calculations flow balance analysis, or they can be used to verify and validate simpler, or perhaps more complex, line pack calculators.

3.2.2 Online Real-Time Applications

The other class of pipeline simulators is the "on-line" simulators often referred to as a real-time transient model (RTTM) which are enable automatic updating of operating data in real time. This becomes possible when the pipeline simulator is integrated with SCADA (Supervisory Control and Data Acquisition) and receives the data at a regular frequency (typically every 5 seconds). The simulator runs in lock-step with the SCADA system to provide an up-to-date detailed view of the hydraulic state of the fluid conditions in pipeline.

Both PAS (Pipeline Application System) and LDS (Leak Detection System) are a detailed real-time transient model. The RTTM provides useful information about the standard volume, mass or energy content of a pipeline. This information tells operators how much product is in the pipeline; it also helps the operator determine how much spare capacity exists within the system (ultimately

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determined by the maximum allowable pressure within a pipeline or system). The pack rate, an additional calculation commonly used on gas systems, determines the change in inventory over a defined time period and reports whether the line is packing or unpacking and at what rate the change is occurring.

3.2.3 Real-Time Pipeline Simulators

PAS is based on a detailed RTTM designed specifically **for decision support**. PAS runs predictive and look-ahead simulations driven by scenarios i.e. prescribed changes in pressure and flow boundary conditions, using the current real-time state as the starting state for the analysis. Typical PAS functionality is Survival Time analysis: based on the current pack rate this analysis provides an estimate of how long a pipeline can run with the loss of a supply or delivery before some system constraint is violated. PAS is a model requiring continuous flow paths from pipeline ingress to pipeline egress with typical boundary conditions being flow at pipeline egress and pressure and temperature at pipeline ingress. As PAS is a decision support system, computational speed is often critical.

LDS is based on a detailed RTTM designed for **accurate, robust, reliable, and sensitive leak detection**. LDS is a real time model only and look-ahead and predictive capabilities are not available by design. LDS provide high spatial resolution and accurate line pack calculation, a necessary requirement for high-fidelity model-based leak detection. Computational speed is not critical for this model and pressure boundary conditions only are in use. Whereas PAS requires continuous flow paths, LDS can model the pipeline as a set of near-independent segments with each segment having pressure boundary conditions. The ability to segment the model in this way enhances the accuracy of the calculated line pack.

PAS and LDS solve the same set of transient flow equations provided in Section 8:

- conservation of mass
- conservation of momentum
- conservation of energy
- equation of state
- radial heat transfer

These flow equations are much more detailed than the simplified Equation (3) and form a coupled system. As the equations are evolutionary their solution depends on two factors: the solution at a previous time and changes in the boundary conditions between the previous and current time. The boundary conditions are typically flows, pressure, temperatures and gas composition for specific points in the network (supplies and deliveries) received from SCADA at a fixed time interval.

The hydraulic and thermal profiles in the pipes are transient in nature and are computed by solving the time-dependent mass, momentum and thermal balance equations. The solution of these equations is undertaken on a numerical grid comprising contiguous and adjoining computational cells within each pipe. The pipeline pressure, flow, velocity, density and temperature are stored at the ends of each computational cell. Typically, the computational cells are 300-400 m in length.

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3.3 PAS and LDS Overview

3.3.1 Configuration

There are many parameters that are required to configure PAS and LDS. The core configuration data is a physical description of the pipeline geometry including, but not limited to, the length and diameter of each of the pipes, the connectivity of the pipes and other in-line equipment and the elevation profile. The configuration will also include details of the stiffness of the pipe walls, the thermal characteristics of both the pipe and the external medium surrounding the pipe. Additionally, a description of the fluids entering the pipeline system is required. Typically, this will be the gas composition and the equation of state used to model the fluid. As SCADA data is used, a careful mapping of the SCADA tags to PAS and LDS must be made.

Some of the parameters required by the model are very difficult to determine with any accuracy, such as the pipe roughness and thermal parameters of the medium external to the pipe. Typically, these parameters are automatically tuned to ensure good agreement between the modelled and measured values.

3.3.2 Measured Inputs

Measurement instruments determine the gas pressure and temperature along the pipeline, gas composition and flow rates at the pipeline inlet and outlet. The same measured values are used as input parameters (boundary conditions or reference values) for both PAS and LDS models. If the measured values are used as boundary conditions to the model, then measurement instrument uncertainty propagates directly to the model state. Therefore, it is important that the measurement instruments are correctly calibrated and maintained regularly.

PAS has limited number of measured values used as input parameters in the model, therefore the uncertainties of measurement instruments are more significant. LDS is designed for robust leak detection and to support this functionality more measurement instruments are required. This results in LDS improved leak detection performance and more accurate line pack calculation than PAS.

3.3.3 Boundary Conditions

The main difference between PAS and LDS is how the pipeline models are constructed. While most of the configuration data is used identically in both, the assignation of boundary conditions is different.



Figure 2 – PAS Boundary Conditions

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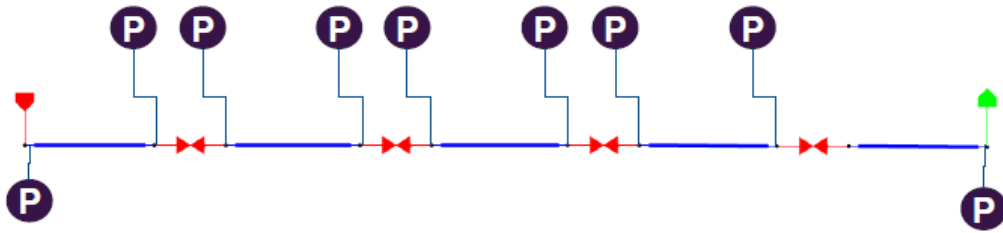


Figure 3 – LDS Boundary Conditions

PAS allows flow or pressure boundary conditions at either end as Figure 2 shows. The pipeline is modelled as a single segment. PAS uses real time pressure, temperature and gas composition data at the pipeline inlet, and flow rate at the pipeline outlet.

LDS permits pressure boundary conditions only as Figure 3 shows. The pipeline is modelled as a series of segments. LDS uses real time pressure, temperature and gas composition data; flow is not included as a boundary condition.

From the point of view of line pack calculations, usage of pressure measurements as boundary conditions is a preferable option. Firstly, pressure and temperature can be measured more accurately than flow. Secondly, pressure and temperature are the key components of the line pack calculation since both density and volume are functions of pressure and temperature. Therefore, LDS provides a better assessment of line pack than PAS.

3.3.4 Complexity (PAS)

Generally, the more detail and complexity that is included in a pipeline model configuration the longer it will take to run. A comparison between a detailed real-time model, where the topology and configuration of the compressor stations match those in the field, and a reduced but logically equivalent model, in which the configuration of the compressor stations is much simplified, has been undertaken for an existing PAS implementation.

With improvement in execution time from 12,960 to 165 seconds for a 72-hour simulation (3-day look ahead), the inventory of the reduced model was found greater than the inventory of the detailed model with the relative difference not exceeding 0.14 %. As previously mentioned, speed is crucial for PAS, and reducing model complexity does not necessarily compromise accuracy.

3.3.5 Spatial and Temporal Resolution

Significant gains in computational performance can often be made by reducing the resolution of the numerical grid associated with each pipe.

Each pipe is divided into a large number of small segments (spatial increments) allowing numerical solution of transient flow equations along the pipe. The smaller the spatial increment, the more accurate the solution will be. Typically for LDS a spatial increment of 250 m is set whereas for PAS it is often around 5000 m.

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Again, for an existing implementation of PAS and LDS, the difference in line pack calculation may reach 1.66 % with a spatial increment of 5000 m and decrease to 0.02 % at 500 m spatial increment as Figure 4 shows.

Reducing the spatial increment increases the time it takes to compute the state in each cycle. Applying the spatial increment of 250 m to PAS increases a 24-hour look-ahead performance time by 20 minutes. A typical requirement of PAS is to perform a 24-hour look-ahead within a couple of minutes, therefore the PAS spatial increment is often set to 5000 m.

Typically, the line pack is calculated every 5 seconds by LDS and every 30 seconds by PAS. As well relying on the spatial increment, the accuracy of line pack calculation also depends on the time step (time between state calculations) as Figure 4 shows. The difference in line pack calculation can be observed at the level of 0.5 % at 5 s and with the time step increase the difference is growing.

Due to smaller spatial increment and time step implemented in LDS, this model is expected to provide a much better estimate of line pack than PAS.

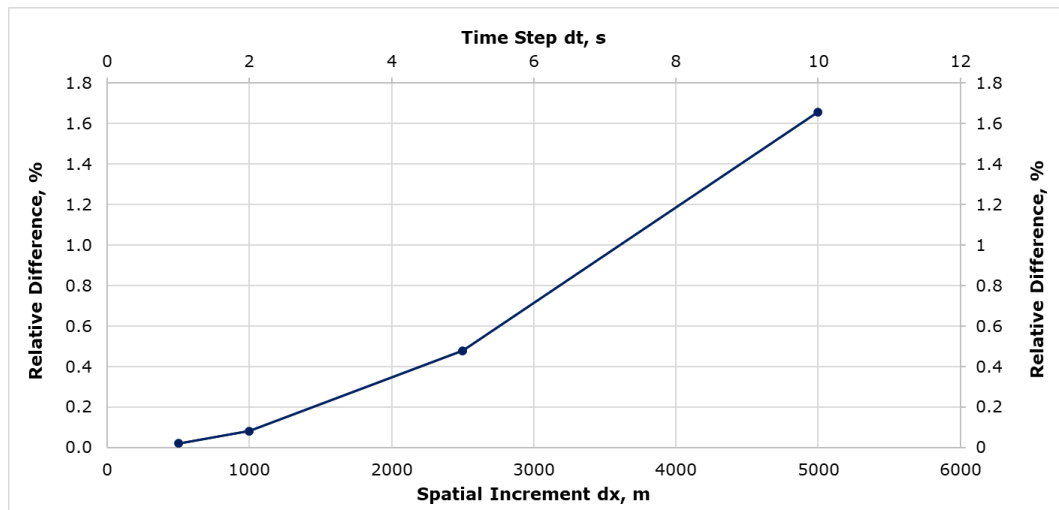


Figure 4 – Effect of Spatial Increment and Time Step

3.3.6 Equation of State

The selection of the equation of state used within the pipeline simulator can significantly impact both accuracy and computational performance.

Comparing the densities computed by GERG-2008, AGA8, BWRS and CNGA for typical sales gas, the diagrams in Figure 5 show the relative differences:

- GERG-2008 vs. AGA8: 0.028 % to 0.056 %
- GERG-2008 vs. BWRS: -0.6 % to 0.23 %
- GERG-2008 vs. CNGA: -3.3 % to -0.46%

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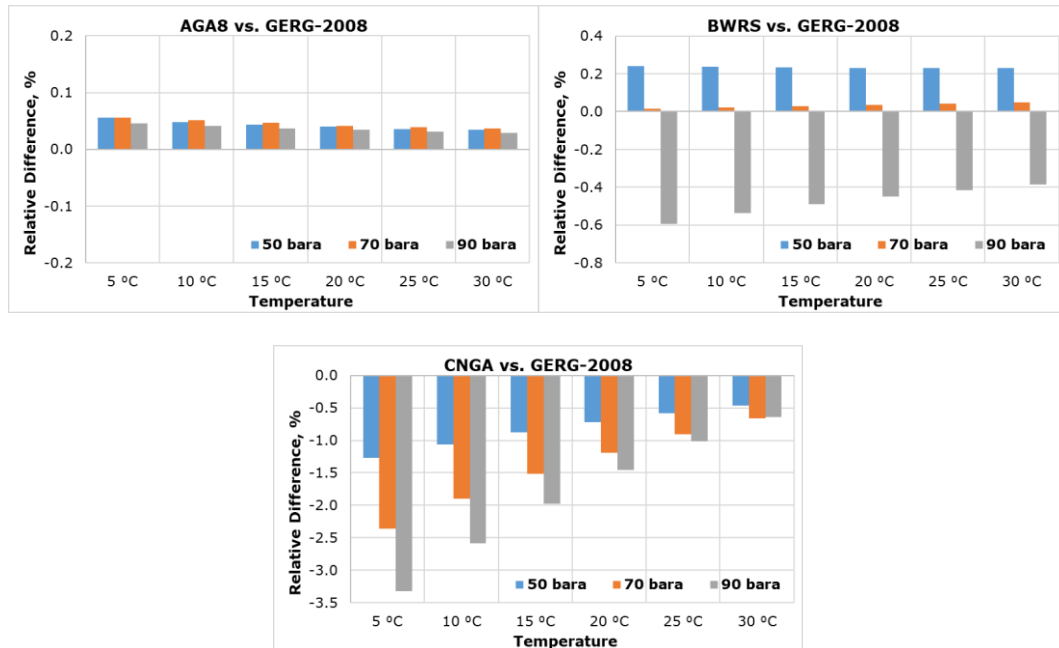


Figure 5 – Equation of State Comparison Results

In terms of computational load, a pipeline simulator requires not just the density to be computed, but 1st (and perhaps 2nd) derivatives of density with respect to pressure and temperature, and isobaric and isochoric specific heats and their densities with respect to pressure and temperature. This requirement is driven by the formulation of the numerical solution of the flow equations.

Furthermore, each of these variables is required within each computation cell in the system. Hence each timestep can see the equation of state being used many thousands of times. If carefully implemented, in most equations of state computational savings can be made by reusing intermediate variables when computing all required properties.

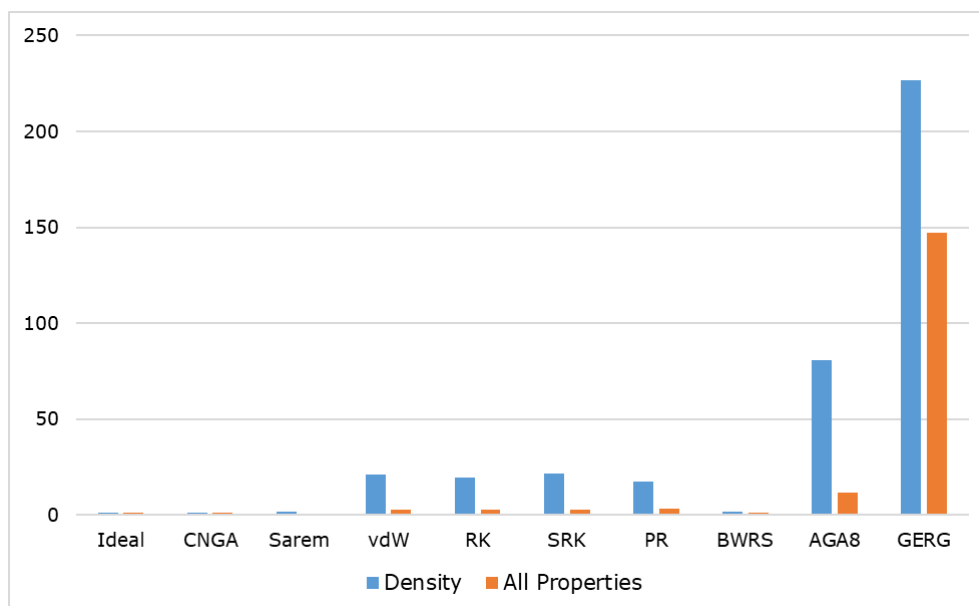


Figure 6 – Relative Computational Intensity of Equations of State

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Figure 6 illustrates a comparison of computational intensity for various equations of state, both separately for density and collectively for all properties. The chart demonstrates that GERG-2008 performs significantly slower, taking 230 times longer for density and 150 time longer for all properties compared to most other equations of state. Typically, AGA8 is approximately 7 times more computationally intensive than BWRS, while GERG-2008 is approximately 100 times more computationally intensive.

Based on our experience, when dealing with moderately complex LDS application that only require real-time performance, GERG-2008 can be a suitable choice. However, for PAS application, GERG-2008, and even AGA8, prove to be excessively computationally expensive.

3.4 Line Pack Calculation Results

The line pack calculation results using three applications (SLP, PAS, LDS) for the selected three-month period are provided in Figure 7. The results exhibit a similar trend, indicating consistency among them. However, the LDS results have shifted from SLP to PAS, with the calculated difference approaching zero.

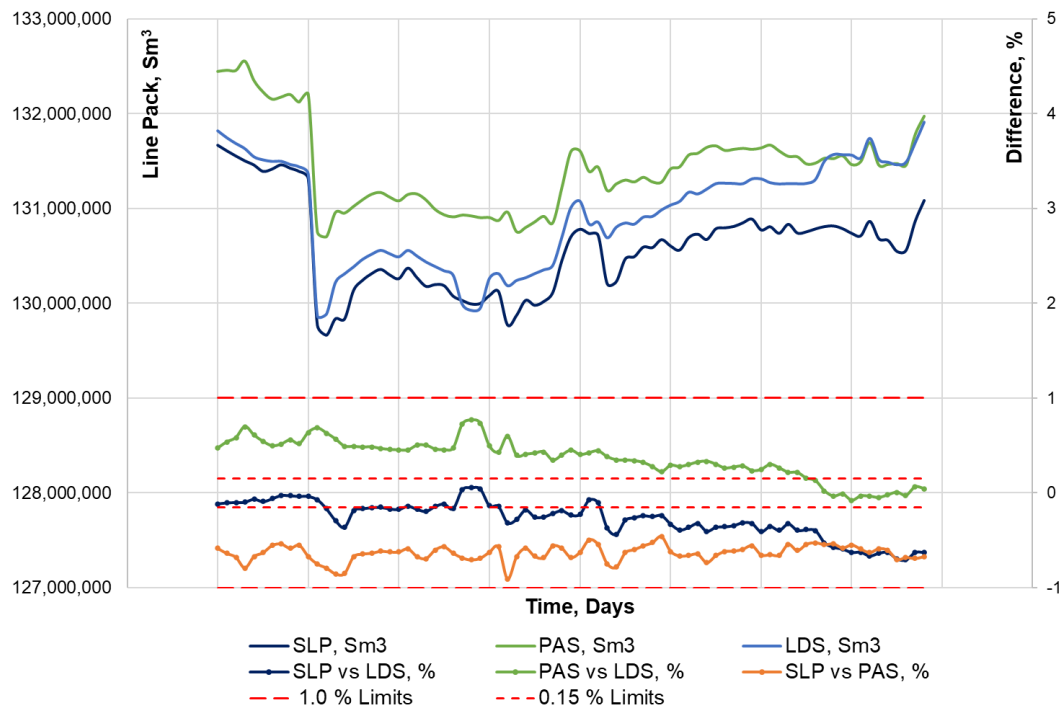


Figure 7 – Line Pack Calculation Results

When both LDS and PAS are initiated, there follows a period when both may experience instability due to the ongoing effects of pre-initiation operational changes.

The calculated line pack values demonstrate an agreement of better than 99 %, or the difference between the values does not exceed ± 1.0 % limits over the selected three-month period for all three calculation methods, as demonstrated in Figure 7. Notably, LDS and PAS, after a period of stabilisation fall, within the

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tighter limits of $\pm 0.15\%$ defined by the line pack uncertainty (refer to Section 3.1).

In summary, the line pack calculations from SLP, PAS, and LDS applications generally follow a similar trend. Consistent monitoring of the line pack values can serve as a quality control measure and help identify operational issues if the difference between calculated line pack values monitored by different applications exceeds a set limit.

3.5 Applications Configuration and Validation

Before implementing any application, it is advisable to validate both configuration and calculations. The validation results, obtained through detailed analysis and comparison with reference software, may reveal an array of potential issues critical for operation.

3.5.1 Common Configuration Pitfalls

The list of common issues, not limited to the points below, is as follows.

Pipeline Configuration:

- Inconsistent pipeline configuration data between the application and design documentation (pipeline diameter, pipe wall thickness variability, elevation, length of segments, number of segments etc..).
- Errors in translation of pipeline geometry into the models. Incorrect interpretation and assumptions of pipeline configuration.
- Omissions of temperature and pressure corrections for pipe inner diameter.
- Valves position is not tracked/recorded. Therefore, the measured parameters are replaced by calculations in the model.
- Configuration and event logs are not maintained.

Measurement Instruments:

- Faults in measurement instruments (pressure, temperature, flow rate, and gas composition) due to lack or absence of maintenance.
- Mismatch between the configured and calibrated ranges of measurement instrument.
- Omissions in calibration of the analogue output of measurement instruments.
- Presence of errors exceeding the permissible limits in the calibration results of measurement instrument.
- Incorrectly configured data sources. Missing tag mapping diagrams showing the data transfer from measurement instruments through SCADA to the model.
- Incorrectly selected resolution of SCADA analogue input blocks for the conversion of the analogue output signals of the measurement instruments.

Model Parameters:

- Incorrect conversion of measured pressure and temperature into absolute values.
- Omissions of variation of gas composition along the pipeline.
- Usage of the default and fixed process parameters (gas composition, pressure and temperature, density, compressibility etc.) instead of real-time values.
- Usage of incorrect model parameters (dynamic viscosity, thermal expansion coefficient, Young's modulus, etc.),

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- Assumption of unknown model parameters (friction factor, overall heat transfer coefficient and other quantities) used for tuning.

The most significant effect on the line pack calculation will be the geometry of the pipeline affecting the volume calculation, both atmospheric and process pressure measurement, and gas compressibility calculation. Errors in these values, together with the issues listed above, may lead to differences in the line pack calculation results and impact immediate operational decisions.

Rectifying the configuration errors is important for preserving operational accuracy and preventing cumulative effects that could potentially affect decision-making over time.

3.5.2 Model Validation with Reference Software

Validation of simulation models is a common practice to ensure their accuracy and reliability in replicating real-world scenarios. One widely used validation method involves comparing the results produced by one simulation tool with those generated by another, provided that both models are configured with the same parameters. The LDS model has been selected for validation, as it was demonstrated to be the most accurate application (refer to Section 3.3).

Validating the entire pipeline model can be a challenging procedure. Therefore, the specific sections of the pipeline may be selected for validation. For instance, results obtained by the in-operation LDS for two inter-block valve sections are suggested for comparison to those obtained from an independent pipeline simulator, such as PipelineStudio (PLS) described in Section 3.2.1. To ensure a fair comparison, PLS is configured with parameters as closely aligned to those of LDS as possible.

PLS has a strong track record among engineers for conducting both steady-state and transient analyses and is the direct descendant of earlier software developed in the 1980s. It has also been employed for calibrating Real-Time Transient Modeling (RTTM) systems and other offline hydraulic simulation tools, making it a suitable benchmark for validation.

Before proceeding with the comparison, two crucial factors needed consideration. Firstly, the in-operation LDS is a transient model that operates continuously, leading to a state of permanent transience. Secondly, the LDS system automatically adjusts several parameters. Typically, these conditions would pose challenges when comparing an online simulator like LDS with an offline simulator like PLS. However, the stability of certain system variables and the relatively short length of the pipeline segments under consideration allow for a reasonable level of agreement between a transient and steady-state simulator.

In addition to validating the LDS results against PLS, an independent analysis to examine the role of tuning in inventory calculations should be conducted. The LDS RTTM can be replayed using archived SCADA data using the same tuning parameters employed on the live system, and with all tuning disabled. The goal is to observe inventory trends and highlight the impact of automatic tuning.

The validation of an in-operation LDS has been conducted and the results of the comparison between PLS and LDS demonstrated the effectiveness of the LDS

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system, despite operating in real-time and online for an extended period, when compared to the steady-state PLS simulator. The inventories computed by LDS and PLS exhibited a high degree of concurrence, with agreement levels of 99.97 % and 99.89 % for two selected sections. Moreover, the correlation between the modelled and measured variables further strengthens confidence in the accuracy of the LDS results, given the configuration parameters and inputs it receives.

3.6 Choosing Between Line Pack Calculation Solutions

Deciding whether to develop an in-house line pack calculation system or use an off-the-shelf solution depends on organization priorities, resources, and long-term goals. Both options have their advantages and disadvantages which are summarised in Table 4 and advantages are highlighted by green colour. It's important to carefully evaluate the specific needs before making a decision. Consider factors such as customization requirements, data privacy concerns, the expertise of your team, budget constraints, and the potential impact on overall operations.

Table 4 – Comparison of Applications for Line Pack Calculation

Aspect	Off-the-Shelf Solution	In-House Solution
Expertise and Best Practices	Built by industry experts with best practices.	Opportunity to build domain expertise.
Speed of Implementation	Quick deployment with pre-built solutions.	Longer development time from scratch.
Accuracy and Reliability	Rigorously tested for accurate results. It is built by experts in the field and designed to handle complex gas dynamics.	Requires thorough validation for reliability. It might be prone to errors if not thoroughly tested or if development team lacks expertise.
Scalability	Scalable for different network sizes.	Scalability may require additional effort.
Continuous Updates	Regular updates to reflect industry changes.	Updates and improvements under internal control.
Technical Support, Maintenance and Updates	Vendor provides technical support, updates, and bug fixes.	In-house team handles support which can be resource intensive and time-consuming.
Resource Intensity	Less internal resource demand.	Requires significant internal resources.
Customization	Limited customization based on vendor offerings.	Highly customizable to meet network needs.
Data Privacy	Concerns about sharing data with third party.	Better control over data security and privacy.
Integration	Integration complexity with existing systems.	Can be integrated seamlessly with existing systems.
Control and Flexibility	Less control over updates and features.	Full control over development, updates, and features.
Knowledge and Skills	Relies on vendor's expertise.	Develops internal knowledge and skills.
Dependency on Vendor	Reliance on vendor for updates and support.	Internal control over updates and support.

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Aspect	Off-the-Shelf Solution	In-House Solution
Cost Efficiency	Licensing or subscription costs over time.	Upfront development cost over time.
Risk of Loss of Expertise	Expertise is retained within the company. However, the solution can be discontinued.	If the in-house developers resign, retire or are transferred to other areas, the invested knowledge in the system can erode over time rendering the tool unsupportable.

4 ALTERNATIVE FLUIDS

Pipeline simulators play a crucial role in the field of CO₂ and hydrogen applications for several reasons. Firstly, they enable engineers and researchers to accurately model the behaviour of these gases within complex pipeline systems. This is essential for optimizing the design and operation of pipelines, ensuring safety, efficiency, and cost-effectiveness.

Furthermore, pipeline simulators are instrumental in assessing the environmental impact of CO₂ and hydrogen transportation. For CO₂, simulators help predict and mitigate potential leaks, reducing greenhouse gas emissions and minimizing environmental harm. In the case of hydrogen, simulators aid in addressing safety concerns by identifying potential hazards and optimizing safety protocols.

Additionally, these simulators are invaluable tools for studying the integration of hydrogen and CO₂ pipelines into existing energy infrastructure, facilitating the transition to cleaner and more sustainable energy sources. They enable thorough analysis of system dynamics, pressure fluctuations, and temperature changes, all of which are critical for reliable and efficient gas transport.

It's worth noting that despite operational similarities between natural gas and alternative fluids, there are unique factors to consider:

- CO₂ can be transported in dense phase, and therefore, compressibility is lower than one would expect with natural gas.
- Blending H₂ into natural gas increases the compressibility.
- Both fluids tend to react with other components, and their thermodynamic properties are very different from typical natural gases.

Provided the fluid model is accurate, the line pack can be precisely calculated for any single-phase fluid. Currently, the LDS is successfully implemented on CO₂ pipelines, demonstrating its effectiveness in practice.

4.1 Carbon Dioxide CO₂

When modelling CO₂ in pipeline simulators [4], several factors need to be considered to ensure accuracy and stability in the calculations. These factors can be summarized as follows:

Availability of fluid property calculation packages. To model CO₂ in pipelines effectively, it is essential to have access to fluid properties.

- LDS/PAS simulators require the density and the first and second derivatives with respect to pressure and temperature, as well as isobaric/isochoric specific

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heat capacities and their first and second derivatives with respect to pressure and temperature.

- AGA8 (only for gaseous state) along with other equations of state (PR, SRK, BWRS, etc.) can be easily implemented.
- GERG-2008 is available via REFPROP, but it is exceedingly computationally intensive (refer to Section 3.3.6).
- EoS-CG 2013 is not commercially available.

Accuracy of CO₂ modelling depends on several factors:

- For pure compositions, fluid property look-up tables based on S&W can be utilized.
- When composition doesn't vary significantly, fluid property look-up tables based on GERG can be used, but caution is needed due to the range of uncertainty.
- If composition varies substantially, direct calculation of fluid properties using GERG is possible, but one must be aware of the computational cost and range of uncertainty. In practice, long and complex pipelines can run in real-time using GERG-2008, but this approach may push the computational limits.

Stability in CO₂ pipeline simulations is crucial. Here are some key considerations:

- Most highly accurate real-time transient multiphase (RTTM) systems for pipeline simulations are designed primarily for single-phase calculations. Multiphase models tend to be significantly less accurate.
- Numerical methods used in these simulations rely on estimating density spatial and temporal derivatives, often computed using the chain rule. Near phase envelopes or boundaries, density derivatives with respect to pressure and temperature can become excessively large, potentially leading to numerical instability in the solver.
- Fortunately, recommended CO₂ pipeline operations involve running in dense/supercritical phases while avoiding multiphase or phase change conditions. This helps maintain stability in the simulations. In dense/supercritical region accuracy of LDS will depend on accuracy of fluid property model.

4.2 Hydrogen H₂

When modelling the behaviour of H₂-enriched natural gas within a pipeline simulator, several key considerations come into play.

Availability of fluid property calculation packages:

- LDS/PAS simulators require the density and the first and second derivatives with respect to pressure and temperature, as well as isobaric/isochoric specific heat capacities and their first and second derivatives with respect to pressure and temperature.
- AGA8 (only for gaseous state) along with other equations of state (PR, SRK, BWRS, etc.) can be easily implemented.
- GERG-2008 is available via REFPROP, but it is exceedingly computationally intensive (refer to Section 3.3.6).

Accuracy. When evaluating the accuracy of these modelling approaches, it's important to consider their performance. AGA8 (detailed) tends to provide a high degree of agreement with GERG-2008 for H₂ concentrations up to 20 % and

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possibly even beyond. However, one limitation of AGA8 is that it is technically not an equation of state because it does not predict the fluid state.

Stability. In practical pipeline operations, the system typically operates well away from the phase envelope. Therefore, the issue of stability is generally not a concern. Nevertheless, it's advisable to include pipeline operations and a phase diagram analysis in modelling efforts to ensure a comprehensive understanding of system behaviour.

Fugitive Emissions. Hydrogen molecules are smaller compared to larger molecules like methane and can more easily permeate through materials, which can make containment and leak prevention more challenging. One of several measures to mitigate the risk of increased fugitive emissions is the advanced leak detection technologies that can quickly identify and locate hydrogen leaks.

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5 CONCLUSION

This paper underscores the significance of comprehending the factors contributing to gas pipeline imbalances. The primary parameters affecting imbalance are noted as the line pack, inlet and outlet volumes, and their dependence including pipeline geometry, atmospheric and process pressure, and gas compressibility.

Setting appropriate imbalance limits based on the flexibility of line pack and the uncertainties associated with measuring instruments is a critical step. These limits should be closely aligned with the capabilities of the hardware and software in use, and they can serve as alarm levels to trigger immediate corrective actions when exceeded.

Imbalance calculations hinge on accurate line pack determinations, which can be achieved through various methods. However, the choice of calculation method (tool, application) should be made with careful consideration and a thorough understanding of their purpose and specifications. Employing robust real-time software packages for line pack calculations enhances precision and efficiency, with the Leak Detection System (LDS) emerging as a highly accurate option. The LDS model has been validated using PLS (refer to Section 3.5.2) with the agreement level better than 99.89 % (or error of 0.11 %).

The evaluation of software development routes, outlining the pros and cons of off-the-shelf applications (refer to Section 3.6). It is clear that there is no one-size-fits-all solution, and the choice should be guided by available resources and specific needs.

While the quality of software plays a crucial role, its accuracy is predominantly shaped by its configuration and input data. It is essential to acknowledge that calculation results are contingent on software configuration, including the equation of state, pipeline geometry, and measurement instruments (refer to Section 3.5.1).

Once in operation, regular validation of the line pack calculation software is imperative, encompassing geometry configuration, condition and calibration results of measurement instrument, tags mapping and signal conversion. This validation ensures that ongoing changes are correctly implemented.

Through meticulous error identification, categorization, and subsequent correction, gas transmission and distribution systems can operate with enhanced precision and reliability.

In the context of transitioning to a net-zero future, the paper has shed light on the considerations for alternative fluids like natural gas-hydrogen mixtures and the transportation of carbon dioxide (refer to Section 4). The availability of fluid property calculation packages, accuracy and stability of software are addressed.

In conclusion, this paper underscores the importance of a comprehensive understanding of gas pipeline imbalances and its limits, emphasizes the need for validation and adaptation of the application in use navigate the evolving landscape of energy transportation.

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6 ABBREVIATIONS

AGA	American Gas Association
BWRS	Benedict-Webb-Rubin equation of state
CAE	Computer-Aided Engineering
CNGA	Californian Natural Gas Association
EOS-CG	Equation of State for Combustion Gases
EU	European Union
GERG	Groupe Européen de Recherches Gazières
GUM	Guide to the expression of Uncertainty in Measurement
LDS	Leak Detection System
LP	Line Pack
PAS	Pipeline Application System
PLS	PipelineStudio
PR	Peng-Robinson equation of state
REFPROP	NIST Reference Fluid Thermodynamic and Transport Properties Database
RK	Redlich-Kwong equation of state
RTTM	Real-Time Transient Model
SCADA	Supervisory Control and Data Acquisition
SLP	Simplified Line Pack
SRK	Soave-Redlich-Kwong equation of state
S&W	Span & Wagner
vdW	van der Waals equation of state

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8 APPENDIX: Pipe Flow Equations

- Mass Balance**

$$\frac{\partial}{\partial t}(A\rho) + \frac{\partial}{\partial x}(Av\rho) = 0$$

- Momentum Balance**

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} + g \frac{\partial h}{\partial x} + \frac{fv|v|}{2D} = 0$$

- Thermal Balance**

$$\rho c_v \left(\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = - \frac{1}{A} T \frac{\partial P}{\partial T} \left(\frac{\partial A}{\partial t} + \frac{\partial}{\partial x}(Av) \right) + \frac{1}{A} P \frac{\partial A}{\partial t} + \rho \frac{fv^2|v|}{2D} - \frac{4U_w(T - T_g)}{D}$$

- Colebrook-White Friction Factor**

$$\frac{1}{\sqrt{f}} = -2 \log \left(\frac{\epsilon/D}{3.7} + \frac{2.51}{Re \sqrt{f}} \right)$$

- Radial Heat Transfer**

To better model heat loss through the pipe wall, the term:

$$\frac{4U_w(T - T_g)}{D}$$

can be replaced by a concentric shell thermal model of the form:

$$\frac{1}{a} \frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r}$$

- Pipe Wall Expansion**

$$A = A_0 e^{Y_s(P - P_0)} e^{\eta(T - T_0)}$$

- Equation of State**

$$\rho = \rho(P, T, c)$$

NOTATION

The symbols defined within the paper are not listed below.

A	m ²	Pipe Cross Section Area
A ₀	m ²	Pipe area (at reference pressure and temperature)
c	mol/mol	Gas composition (detailed characterisation)
c _v	KJ /Kg/ K	Specific Isochoric Heat Capacity of gas
D	m	Pipe inner diameter (at line pressure and temperature)
f	-	Moody (Darcy-Weisbach) friction factor
g	m/s ²	Acceleration due to gravity
h	m	Pipe elevation
P	Paa	Absolute Gas Pressure
P ₀	Paa	Absolute Reference Pressure
r	m	Shell radius (from centre of pipe)
Re	-	Reynolds number

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t	s	time
T	K	Gas Temperature
T_0	K	Reference Temperature
T_G	K	Ground temperature
U_w	W/m ² K	Overall Heat Transfer Coefficient
v	m/s	Gas velocity (Eulerian)
x	m	Distance along pipe
α	m ² /s	Thermal diffusivity
γ_s	Pa ⁻¹	Pipe material stiffness
ε	m	Absolute Roughness
η	K ⁻¹	Pipe thermal expansion coefficient
θ	K	Shell temperature
ρ	kg/m ³	In-situ gas density
$\left(\frac{\partial P}{\partial T}\right)\bigg _{\rho}$	Pa/K	Rate of change of pressure with respect to temperature at constant density