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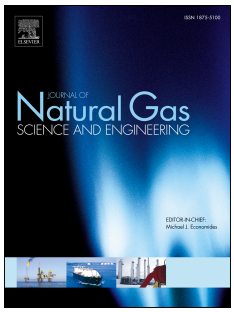


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ACCEPTED MANUSCRIPT

# Gas composition tracking in transient pipeline flow

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**Abstract**

Tracking changes in gas composition in natural gas pipeline transport systems is becoming increasingly important to pipeline operators, since gas suppliers are shifting from long-term delivery contracts to shorter-term contracts, increasing delivery of gases from unconventional sources, and proposing to inject hydrogen and biomethane into the natural gas networks. The present study investigates two methods for tracking gas composition, one using a moving grid method, and one solving the advection equation using an implicit backward difference method. The methods were applied to a model of an onshore pipeline in the Polish transmission system, and a model of an offshore pipeline in the Norwegian transmission system. The differences between the measured and modeled compositions and transport times were investigated. Both methods reproduced the measured compositions and transport times well, with an error in total transport times of less than 2.0 %. The implicit method was found to lose some of the finer details of the gas composition profiles due to numerical diffusion, while the moving grid method preserved the composition profiles.

*Keywords:* Natural gas pipeline, Transient non-isothermal flow, Gas quality tracking, Advective mass transport, Pipeline flow simulation, Implicit method

## 1. Introduction

Transient analyses of flows and pressures in gas pipelines are valuable tools in planning pipeline system reinforcements and operations. Typical transient studies include starting-up/shutting-down compressor stations, linepack management, leak detection and localization analyses, system operation scenarios, gas composition tracking for energy delivery estimation, and flow assurance studies. Gas composition tracking in the pipeline system can be

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**Nomenclature**

| | | |
|---|---|---|
| $A$ | [m$^2$] | Cross-sectional area of pipeline |
| $A_h$ | [m$^2$] | Area through which heat transfer occurs (pipe surface) |
| $c_i$ | [%] | Composition in batch $i$ |
| $C_j$ | [%] | Composition at grid point $i$ |
| $c_v$ | [J/kgK] | Specific heat capacity at constant volume |
| $d_j$ | [m] | Position of grid point $i$ |
| $D$ | [m] | Inner diameter of pipeline |
| $e$ | [m$^2$/s$^2$] | Internal energy per unit mass |
| $f$ | [-] | Friction factor |
| $\dot{m}$ | [kg/s] | Mass flow rate |
| $p$ | [Pa] | Pressure |
| $R_\mathrm{s}$ | [J/kgK] | Specific gas constant |
| Re | [-] | Reynolds number |
| $T$ | [K] | Temperature |
| $u$ | [m/s] | Gas velocity |
| $u_j$ | [m/s] | Gas velocity in grid cell $i$ |
| $x_i^n$ | [m] | Position of batch $i$ at time-step $n$ |
| $Z$ | [-] | Compressibility factor |
| | | |
| $\epsilon$ | [m] | Sand grain equivalent roughness |
| $\theta$ | [rad] | Pipe inclination |
| $\rho$ | [kg/m$^3$] | Density |
| $\Omega$ | [W/m] | Heat flow per unit length of pipe |

considered as an important element of a decision making framework of pipeline operation. In applications like energy delivery estimations or flow assurance studies, it is necessary to track quantities of natural gas mixture constituents or contaminants such as water, hydrogen sulfide or carbon dioxide. These impurities are important due to their corrosion properties, hydrate formation abilities, and effects on contractual obligations. Furthermore, accurate estimation of transport times in gas pipelines ensures exact knowledge of the gas quality at all locations of interest in the pipeline system. In fact, any property that moves at local gas velocity such as gas batches or even a pig traveling through the pipeline may be referred to and treated as a quality [1]. This minimizes the need to mix gases to meet quality specifications as well as mobilization times for manpower. Scenarios where injecting biogas or hydrogen into pipelines traditionaly transporting natural gas also require accurate knowledge of the gas composition or the gas quality in the form of the calorific value of the gas delivered to the end users [2, 3]. To achieve this it is necessary to have an accurate model of the system with a suitable numerical solution scheme.

The governing equations for pipeline gas flow express mass, momentum and energy conservation laws. Additional relations resulting from the introduction of the variables describing the gas composition express processes of advective mass transport. In addition to improving the description of the system, the numerical solution and the input parameters of a pipeline model can also be improved by making use of how the computer model compares to measurement data [4].

An important aspect of any pipeline model is the interaction between the pipeline and the surrounding environment. Depending on how the pipeline is situated on the ground, different accuracies in the heat transfer model might be needed [5]. With regards to the description of the ambient temperature, the quality of available temperature measurements might vary. In the case of subsea pipelines the choice might stand between using average of historical values or making use of model based sea temperatures [6, 7]. To accurately model the gas temperature in buried pipelines it has been shown that a one-dimensional radial model [5] is sufficient to capture the temperature development in the pipeline wall and surrounding ground [8, 9].

The problem of gas quality control under steady-state conditions was studied by van der Hoeven [10]. A steady-state pipeline gas flow model incorporating energy flow was formulated and the simulation of the process of gas blending in which the quality of a mixture was the flow weighted mean of the qualities of the constituent gases was performed. The amount of gas a demand requires was given in energy per time unit instead of standard volume per time unit, therefore the pressure drop equation need to be reformulated in terms of energy flow. At a first glance the simulation of blending of gases seemed to be not difficult, but some convergence problems in the steady-state simulation of such pipeline systems occurred [11]. More recent research studies on gas quality control under steady-state conditions can be found in Schley et al. [12] and Abeysekera et al. [13]. In the earlier study, volumetric flow rate was used as a demand data, while in the later study demand was expressed in energy per unit time.

The need for gas composition tracking under transient conditions rises, since growing LNG markets and renewable gas markets (biogas injections, hydrogen injections pilot plants) lead to increasing gas quality variations in the grids, while at the same time more stringent requirements are coming from regulators demanding harmonised rules in the area of gas quality in Europe. The challenges brought by these evolutions are of particular interest for transmission system operators, which are responsible for coordination of gas deliveries.

In their publication, Ryan and Mailloux [1] focused on presentation of the two composition tracking methods, namely the implicit method incorporating upwind finite difference scheme and the explicit random choice method, the later involving the solution of the Riemann problem [14]. The two methods were compared and contrasted by changing the inlet quality parameter (calorific value and specific gravity) with time, and observing the changes in time along the pipeline. The results demonstrated the numerical diffusion problem associated with the finite difference method. It was also recognized that the sharp interfaces in the quality parameter profiles can lead to oscillations in the solution by the random choice method. The upwind finite difference scheme was also used for calorific value tracking in a state reconstruction problem considered by Hager et al. [15]. More recently, the isothermal

flow of gas with calorific value tracking downstream the injection point of hydrogen in a 50-km-long section of the regional gas transmission system has been investigated by Guandalini et al. [2], and in [16] the effect of simplified steady state heat transfer model on gas quality tracking results and transport times in onshore pipelines was discussed by the authors.

In contrast to the above studies, the present work attempts to evolve the gas composition tracking methodology by using the fully implicit finite-difference method to solve the continuity, momentum, energy equations coupled with mass transport equation for the flow within a gas pipeline. This methodology provides more detailed description of the flow by considering the nonisothermal flow model with heat transfer processes between the gas in the pipe and the surrounding environment, while the fully implicit finite-difference method offers the advantage of guaranteed stability for a large time step, which is very useful for pipeline simulation industry.

The mass transport equation is considered in Eulerian coordinates (implicit method with backward finite difference scheme) and in Lagrangian coordinates (batch tracking method). The two solution techniques are compared by observing the profile of gas composition changes as it travels down the pipeline. The evaluation is based on comparing simulation results to operational data. The investigations are carried out for one pipeline of the Polish onshore gas transmission system, as well as one subsea pipeline in the Norwegian gas export system.

This article is structured as follows. Section 2 presents the theoretical foundation and underlying equations. The numerical scheme is presented in Section 3 followed by the presentation of the studied pipeline systems in Section 4. Results are presented in Section 5 and discussed in Section 6 while concluding remarks are drawn in Section 7.

## 2. Theory

### *2.1. Conservation laws / governing equations*

The governing equations for one-dimensional, non-isothermal, transient pipeline gas flow are: the **continuity equation**

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \tag{1}$$

the **momentum equation** [17]

$$\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) + \frac{\partial p}{\partial x} = -\frac{f \rho \left| u \right| u}{2D} - \rho g \sin \theta, \tag{2}$$

and the **energy equation** [18]

$$\rho \left( \frac{\partial e}{\partial t} + u \frac{\partial e}{\partial x} \right) + p \frac{\partial u}{\partial x} = \frac{f \rho u^3}{2D} + \frac{\Omega}{A_h}, \tag{3}$$

Using a real gas equation of state

$$\frac{p}{\rho} = Z R_{\mathrm{s}} T \tag{4}$$

and introducing the mass flow rate $\dot{m} = \rho u A$, the governing equations are developed into partial differential equations for $p$, $\dot{m}$ and $T$

$$\frac{\partial p}{\partial t} = \left(\frac{1}{p} - \frac{1}{Z}\frac{\partial Z}{\partial p}\bigg|_T\right)^{-1}\left[\left(\frac{1}{T} + \frac{1}{Z}\frac{\partial Z}{\partial T}\bigg|_p\right)\frac{\partial T}{\partial t} - \frac{ZR_sT}{pA}\frac{\partial \dot{m}}{\partial x}\right] \tag{5}$$

$$\begin{aligned}\frac{\partial \dot{m}}{\partial t} = {} & \frac{\dot{m}ZR_sT}{pA}\left[-2\frac{\partial \dot{m}}{\partial x} + \dot{m}\left(\frac{1}{p} - \frac{1}{Z}\frac{\partial Z}{\partial p}\bigg|_T\right)\frac{\partial p}{\partial x} - \dot{m}\left(\frac{1}{T} + \frac{1}{Z}\frac{\partial Z}{\partial T}\bigg|_p\right)\frac{\partial T}{\partial x}\right] \\ & - A\frac{\partial p}{\partial x} - \frac{fZR_sT\dot{m}\,|\dot{m}|}{2DAp} - \frac{pA}{ZRT}g\sin\theta\end{aligned} \tag{6}$$

$$\begin{aligned}\frac{\partial T}{\partial t} = {} & -\frac{\dot{m}ZR_sT}{pA}\frac{\partial T}{\partial x} - \frac{\dot{m}\left(ZR_sT\right)^2}{pAc_v}T\left(\frac{1}{T} + \frac{1}{Z}\frac{\partial Z}{\partial T}\bigg|_\rho\right) \\ & \times\left[\frac{1}{\dot{m}}\frac{\partial \dot{m}}{\partial x} + \left(\frac{1}{T} + \frac{1}{Z}\frac{\partial Z}{\partial T}\bigg|_p\right)\frac{\partial T}{\partial x} - \left(\frac{1}{p} - \frac{1}{Z}\frac{\partial Z}{\partial p}\bigg|_T\right)\frac{\partial p}{\partial x}\right] \\ & + \frac{f}{2c_vD}\left(\frac{ZR_sT|\dot{m}|}{pA}\right)^3 + \frac{ZR_sT}{pc_v}\frac{\Omega}{A_h}.\end{aligned} \tag{7}$$

This hydraulic model, including the closure relations given in Section 2.2 has been calibrated under different operating conditions for both onshore and offshore pipelines [19, 20].

### *2.2. Closure relations*

To calculate the heat transfer $\Omega$ between the gas and the surroundings a transient one-dimensional radial model [5] is used. This model includes heat storage in the pipeline wall and surroundings, which is essential to accurately predict the gas temperature [5, 8]. This heat transfer model has been shown to accurately reproduce measured outlet temperatures [6, 7, 19], but depend on detailed knowledge of the surroundings of the pipeline, like burial depth and the density and other properties of the burial medium.

The GERG-2004 equation of state [21] is used to determine the gas density, the compressibility factor $Z$ and its derivatives, and is also used to calculate properties like the heat capacity $c_v$. GERG-2004 is explicit in Helmholtz free energy [21]

$$\alpha(\delta,\tau) = \alpha^0(\rho,T) + \alpha^r(\delta,\tau), \tag{8}$$

where $\delta$ is the reduced density $\delta = \rho/\rho_c$ ($\rho_c$ is critical density), $\tau$ is the inverse reduced temperature $\tau = T_c/T$ ($T_c$ is critical temperature), $\alpha^0$ represents the properties of the ideal gas, and $\alpha^r$ is the residual part. The compressibility is determined from

$$Z = \frac{p(\delta,\tau)}{\rho R_sT} = 1 - \delta\alpha^r_\delta, \tag{9}$$

where $\alpha^r_\delta$ is the derivative of the residual part of the reduced Helmholtz free energy $\alpha^r$ with respect to reduced density

$$\alpha^r_\delta = \left.\frac{\partial \alpha^r}{\partial \delta}\right|_\tau . \tag{10}$$

This derivative, and the equations for calculating heat capacities, speed of sound etc. is given in [21]. For high pressures, such as in the Norwegian export network, the selection of the equation of state can have a significant impact on the simulation results [19, 22].

The Colebrook-White equation [23] is used to calculate the Darcy friction factor $f$

$$\frac{1}{\sqrt{f}} = -2\log\left(\frac{\epsilon}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right). \tag{11}$$

This implicit equation is solved using the Newton-Rhapson method.

### *2.3. Transport equation*

The transport of any physical quantity by convection and diffusion is described by the convection-diffusion equation. For mass transfer of a species with concentration $c$ and velocity $u$ in a pipeline this has the form

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + D_x\frac{\partial^2 c}{\partial x^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(rD_r\frac{\partial c}{\partial r}\right) = R. \tag{12}$$

Here $u\frac{\partial c}{\partial x}$ describes advection along the pipeline, $D_x\frac{\partial^2 c}{\partial x^2}$ axial diffusion, $\frac{1}{r}\frac{\partial}{\partial r}\left(rD_r\frac{\partial c}{\partial r}\right)$ radial diffusion, and $R$ is a source term for creation or production of $c$. For flow problems in gas pipeline systems the two diffusion terms are very small, and there are no source or sink terms $R$, therefore Eq. (12) reduces to the *advective transport equation* [1]

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0, \tag{13}$$

where $u$ is the gas velocity. In the present study the advective transport equation is used to model the transport of gas components, and to estimate arrival times of peaks in gas quality.

## 3. Numerical scheme

### *3.1. Implicit method for the conservation equations*

The governing equations (Eqs. (5–7)) are discretized using a implicit backward difference method [24]

$$\frac{\partial y(j, t_{n+1})}{\partial t} = \frac{y^{n+1}_{i+1} + y^{n+1}_i - y^n_{i+1} - y^n_i}{2\Delta t}, \tag{14}$$

with first order scheme

$$\frac{\partial y(j,t_{n+1})}{\partial x} = \frac{y_{i+1}^{n+1} - y_i^{n+1}}{\Delta x}, \tag{15}$$

$$y(j,t_{n+1}) = \frac{y_{i+1}^{n+1} + y_i^{n+1}}{2} \tag{16}$$

where $y(j,t_{n+1})$ is the dependent variable (pressure, temperature, mass flow rate and gas composition) at pipe section $j$, and the superscript $n+1$ indicates time level $t_{n+1}$, and the subscript indicates position (or grid point). The resulting system of non-linear equations is linearized about the previous time step, and solved using the Jacobi iterative method.

It needs to be stressed that when considering practical implementation of the implicit method, its numerical efficiency can be significantly increased by selecting appropriate dependent variables for the flow model, as presented for the isothermal flow conditions in the study by Wang et al. [25]. The linearization of the resulting system of equations was achieved by expansion of the nonlinear terms of partial differential equations in a Taylor series and keeping the first order terms only.

### *3.2. Numerical schemes for the transport equation*

Two different numerical schemes were used for tracking gas composition. The first one solves the advection equation in Eulerian coordinate system, as described in Section 3.2.1, and the second one uses a Lagrangian coordinates-based batch tracking method described in Section 3.2.2.

#### *3.2.1. Implicit scheme*

The advection equation (Eq. (13)) is discretized using Eq. (14) and Eq. (15). The resulting system of non-linear equations is solved using the Jacobi iterative method.

#### *3.2.2. Batch tracking method*

When solving the conservation equations with convection terms, problems with numerical diffusion of sharp temperature or composition fronts usually appear [26]. An alternative approach for tracking changes in gas composition is a moving grid method called *batch tracking* [26, 27] which avoids the numerical problems associated with convection.

A *batch* is defined as a fluid element with constant composition $c_i$, located between points $x_i$ and $x_{i+1}$ in the pipeline. The pipeline is discretized into $N$ grid points $d_j$, and $N-1$ *grid cells* (the space between each grid point), as part of the routine for numerically solving the governing equations. Batch positions $x_i$ and grid positions $d_j$ are illustrated in Fig. 1.

The batch tracking algorithm used in this study can be summarized as follows:

- The system can be initialized with one large batch filling the entire pipeline, or for example by assigning one batch to each grid cell.

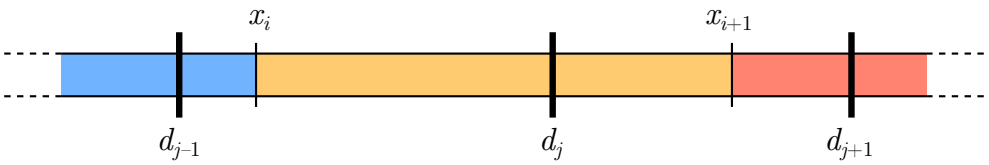


Figure 1: Illustration of batch positions $x_i$ and grid points $d_j$ used in the batch tracking algorithm. The color illustrates different gas composition in each batch.

- The position of a batch $x_i$ at the next time step is calculated as follows

$$x_i^{n+1} = x_i^n + u_j^n \Delta t, \tag{17}$$

where $u_j$ is the velocity of the gas in the grid cell which $x_i^n$ is located in ($d_j \leq x_i^n < d_{j+1}$). The gas velocity $u$ is assumed to be positive in this version of the algorithm, but the algorithm can be modified to accept negative velocities.

  - Special care has to be taken when a batch moves beyond the grid cell it was located in (if $x_i^{n+1} \geq d_{j+1}$). In that case the position can either be calculated using Eq. (17) as before, or accuracy can be improved by dividing the translation into two (or more) steps, one step for each grid cell it moves through. For movement through two grid cells ($d_j$, $d_{j+1}$) and ($d_{j+1}$, $d_{j+2}$) the position at the next time step can be calculated using

$$x_i^{n+1} = x_i^n + u_j^n \Delta t' + u_{j+1}^n (\Delta t - \Delta t'), \tag{18}$$

where

$$\Delta t' = \frac{d_{j+1} - x_i^n}{u_j^n}. \tag{19}$$

This concept can easily be extended for translation through more grid cells.

- At each time step a batch is inserted at the inlet of the pipeline, with composition equal to the inlet boundary condition and position $x_0 = d_0$.
- Finally, the composition $C_j$ at each grid point $d_j$ has to be sampled. In this work the composition of batch $i$, $c_i$, is used, where $i$ is such that

$$x_i \leq d_j < x_{i+1}. \tag{20}$$

An alternative approach is to average over several batches, or interpolate between batches, depending on the number of batches compared to the number of grid grid points.

The batch tracking concept sketched above can easily be extended to more than one quantity, for example for tracking several gas components, by using composition $\vec{c} = (c_0, c_1, \ldots, c_n)$, where $n$ is the number of components.

Although the batch tracking method avoids the problems of numerical diffusion, a different source of error is that the position changes of the gas batches are calculated using dead reckoning (Eq. (17)); each estimate of the batch positions is relative to the previous one, therefore errors in the batch positions are cumulative and will grow with time as the batches move downstream.

## 4. Pipeline systems

This study looks at two different pipeline transport systems, the Polish gas transmission system and the Norwegian export system. The systems serve different purposes and as such have different modes of operation. The Polish system is land based, while the Norwegian system is offshore. This results in two systems operating at different pressures and flow rates, as well as having differences when it comes to design and availability of measurements.

### *4.1. Onshore pipeline*

The Polish gas transmission system connects 67 input points with 983 exit points. It relies on 15 compressor stations to transport 16.3 bcm (183.9 TWh) of gas in high methane and low methane pipelines. The network is operated by a state-owned company designated as a Transmission System Operator (TSO). The company operates 10 989 km of pipelines, primarily transporting high methane gas and mainly concentrated in the south and southwest of the country.

For the analysis of an onshore system the input data from an 81.5 km-long connecting pipeline of an underground gas storage was chosen. This pipeline exhibits satisfactory instrumentation capability for model validation, with both gas flow rate and gas composition measurement data available at entry and exit nodes. The pipeline has an inner diameter of 693.8 mm (28 inches), and the pipeline has no branches or compressors between the measurement points.

### *4.2. Offshore pipeline*

The Norwegian gas export system consists of 8300 km of pipelines. From locations in Norway more than 100 bcm of natural gas is transported to terminals in continental Europe as well as in the United Kingdom each year [28]. The pipelines are for the most part situated, with varying degre e of burial, on the seabed of the North Sea. The subsea location of the pipelines makes it less feasible to have compressor and metering stations along the pipeline. As such the pipelines are typically operated on high inlet pressure without any compressor or metering stations on the seabed.

For the present study all analysis of an offshore system is based on a single pipeline in the North Sea. The pipeline has an inner diameter of 1016 mm (40 inches) and a length of 839.3 km. The pipeline has no branches, no compressors are located between the measurement points, and all valves were fully open in the investigated time periods. The pipeline

model is based on as-laid recordings of burial depths, positions, soil data etc., gathered during pipeline installation and from ROV surveys.

## 5. Results

### *5.1. Onshore pipeline*

In this section gas composition tracking in an onshore pipeline operated during winter months with constant temperature boundary conditions is presented. The simulations were performed using 6-day time horizon with 5-minutes time resolution of the input data, which is typical for current dispatch practices. The roughness of the model ($\epsilon$ in Eq. (11)) was tuned to match the measured pressure drop in the pipeline.

The following boundary conditions were assigned for model validation: the time evolution of outlet mass flow rate, inlet pressure, and inlet concentration of ethane. The model was tracking every gas component and ethane concentration was selected only for illustrating the model validation results. The pipeline was at constant inlet temperature and constant ambient temperature during the simulated period. The input data are shown in Fig. 2. Figure 2 also shows the time evolution of the outlet concentration of ethane used for model validation, which follows the shape of inlet concentration profile with certain time delay resulting from the nature of advective transport. Due to velocity changes over time, transport time varies, as is visible in the different time delays between transients at the inlet and outlet at 34 h and 57 h, at 75 h and 80 h, and at 112 h and 127 h in Fig. 2. The small differences between the measured values at pipeline inlet and pipeline outlet can be attributed to the uncertainty in gas composition measurements.

The numerical discretization errors were investigated for this problem by calculating the local discretization error defined as

$$e = \frac{1}{N}\left[\sum_{i=1}^{N}\left(\frac{Y_i - Y_{i,h}}{Y_{i,h}}\right)^2\right]^{1/2}, \tag{21}$$

where $Y_i$ represents values of flow variable point $i$, while $Y_{i,h}$ is the numerical solution for the respective variable computed using the finest grid (high resolution solution). Fig. 3 shows errors for pressure, mass flow rate and ethane concentration as a function of grid points. The summation is done over all grid points and averaged over time. The local errors are in general small compared to values of the variables. Local error convergence rates for pressure and mass flow rate are slightly lower compared to convergence rate for ethane concentration. A grid density of 80 sections was found sufficient for this particular problem.

Figure 4 shows the predictions of the outlet concentration of ethane using the advective transport model (Eq. (13)) and the batch tracking method. In general, the changes in concentration of ethane propagate along the pipe at correct speed, except for the first 24 hours. This effect can be attributed to the uncertainty of the initial conditions obtained by the steady-state solution of the flow model. Figure 4 also shows that the time rate of change in ethane concentration predicted by the model is slightly lower than that of the measured values, with batch tracking method performing somewhat better than implicit method.

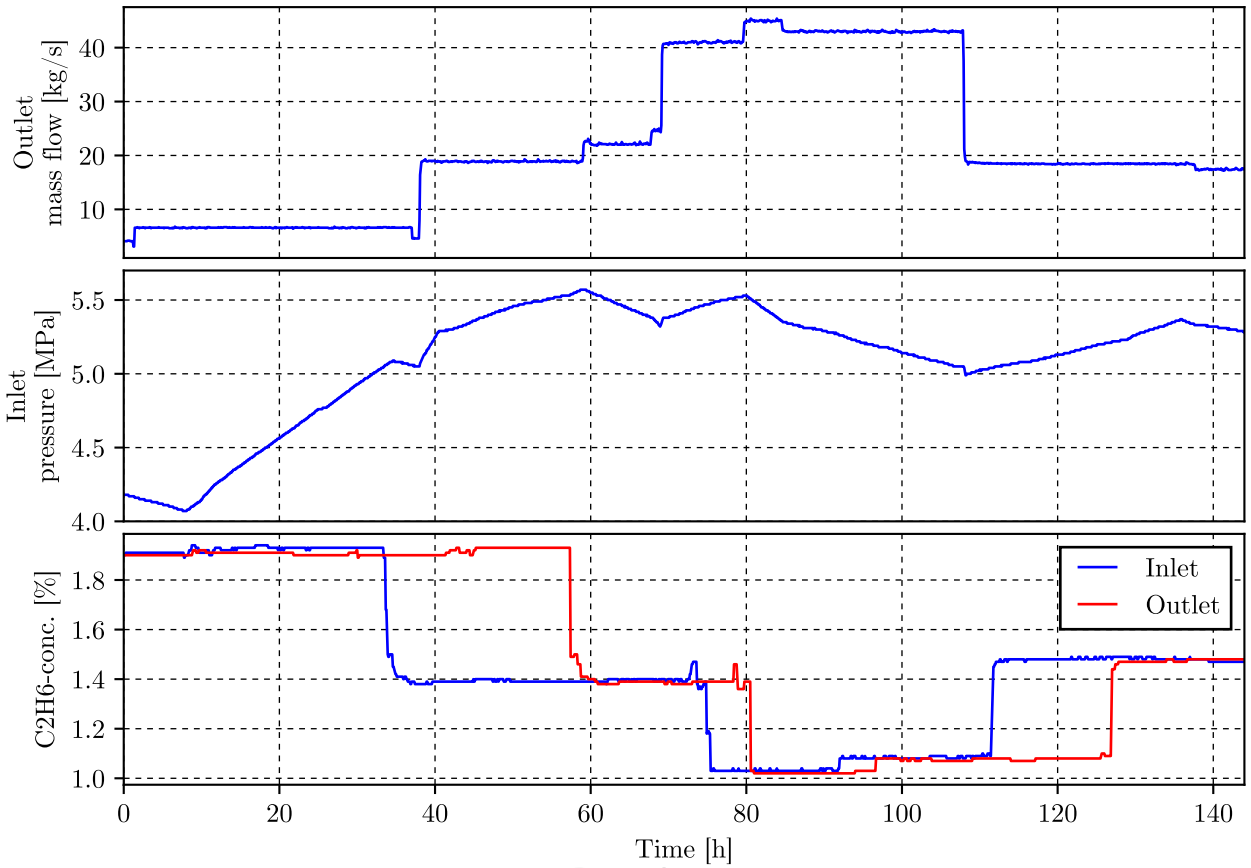


Figure 2: Plot of the boundary conditions used for the onshore pipeline.

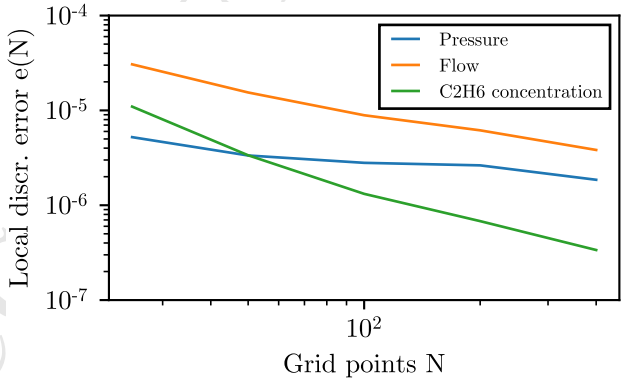


Figure 3: Local discretization error $e(N)$ for pressure, mass flow rate and ethane concentration as a function of grid points $N$.

Turning to Fig. 5 the close-up views of the predictions of the outlet concentrations of ethane for the periods of rapid changes in gas composition show that the numerical solution by the implicit method lags behind the telemetry data, i.e. it is spread out in time, whereas the batch tracking approach eliminated this problem. The observation of the shape of

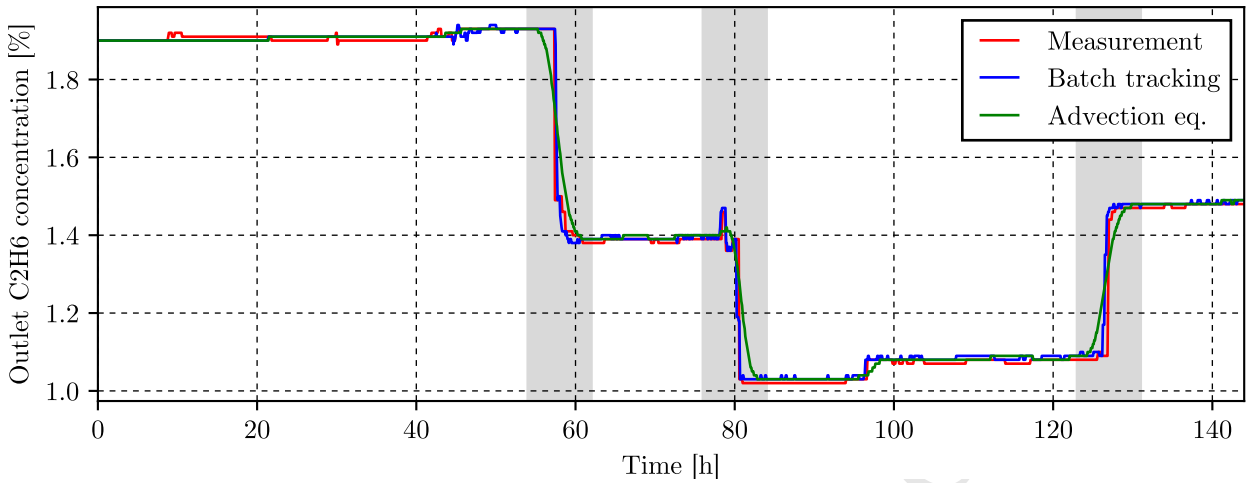


Figure 4: Plot of the measured and modeled outlet $C_2H_6$-concentration for the onshore pipeline. The gray shaded areas are shown in more detail in Fig. 5.

the numerical solution to the left of the step change for the period corresponding to the elapsed time of around 80 hours (Fig. 5B) reveals large distortion of the solution by the implicit method compared to batch tracking method, which precisely follows the shape of propagating discontinuities. The numerical solutions and telemetry data are in slightly better agreement for the elapsed time of around 60 and 130 hours, as indicated in Fig. 5A and C. Clearly, the time rate of change of ethane concentration by the implicit method is significantly underestimated, which makes this method incapable of handling steep slopes. Both methods produce similar discrepancies in the predictions of the estimated time of the arrival (ETA). The error in the predicted transport time was found to be between 10 and 25 minutes. Given that the average transport time was 23 hours, the relative error ranged from 0.7 % to 1.8 %. The differences between the measured arrival times and the arrival times modeled using batch tracking become larger for the latter periods, as seen in Fig. 5.

### *5.2. Offshore pipeline*

The boundary conditions for the offshore pipeline were inlet mass flow, outlet pressure, inlet temperature and inlet $CO_2$-concentration, and the measurement data used as boundary conditions are shown in Fig. 6. The pipeline was simulated for a 14 day winter period and a 18 day summer period. The boundary conditions for the heat transfer model were sea bottom temperature and air temperature profiles along the pipeline that were sampled once per day. The ambient sea bottom temperatures were taken from oceanographic models, and the air temperatures were expected temperatures based on historical measurements.

The ambient temperature was tuned by a constant term along the whole pipeline to match the measured outlet temperature, and the roughness of the model ($\epsilon$ in Eq. (11)) was tuned to match the measured pressure drop in the pipeline. A grid spacing of 1 km and a time step of 60 seconds was found to sufficiently resolve the details in these simulations. At higher grid spacing spurious oscillations in the modeled concentrations occur when large step changes in concentrations are introduced.

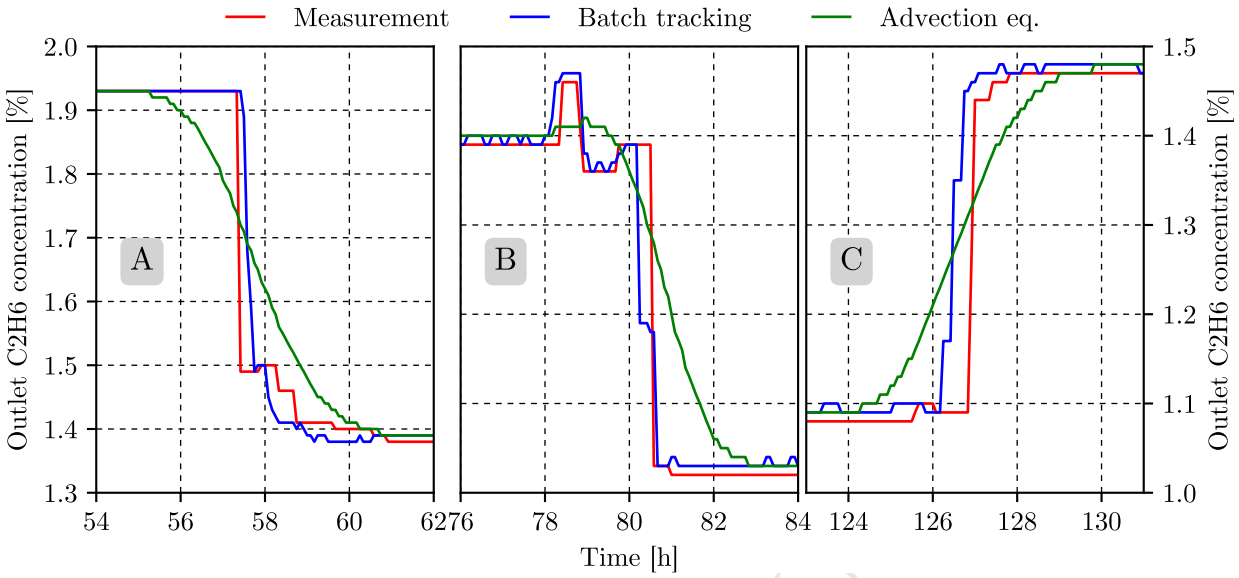


Figure 5: Details of the measured and modeled outlet $C_2H_6$-concentration for the onshore pipeline shown in Fig. 4.

See Figs. 7 to 10 for plots of the modeled outlet $CO_2$-concentration for the both the winter and the summer case. The discrepancies between modeled and measured $CO_2$-concentration between 0 and 50 to 75 hours visible in Figs. 7 and 9 are due to the concentration of the gas present in the pipe at the start of the simulations. The small differences in concentration observed for example around 150-175 hours in Fig. 9 are most likely due to errors in the concentration measurements used as boundary conditions at the pipeline inlet.

In Figs. 7 and 9 it is seen that the modeled outlet $CO_2$-concentration follows the measurements very well on a scale of around 5 hours. The details shown in Figs. 8 and 10 highlight some of the inaccuracies of the modeled results, and it is clear that the finer details of the composition profile are lost when using the implicit method, compared to the batch tracking method which fully preserves the profile. The plots also show that there is an error in the predicted transport time, which is found to be around an hour for the winter case and between 5 and 15 minutes for the summer case. The average transport time is found to be around 50 hours for the winter case and 75 hours for the summer case, giving an error of approximately 2.0 % for the winter case and between 0.1 % and 0.3 % for the summer case.

In Fig. 11 is a plot of the time development of pressure and velocity in the pipeline, at 5 selected positions along the pipeline, for the summer case. This illustrates the transient nature of typical operating conditions, and the velocity development (the right plot) shows the need for a sophisticated hydraulic model to accurately capture the details of the variations in the gas velocity in compressible flows, which is needed to accurately track composition changes in the pipeline.

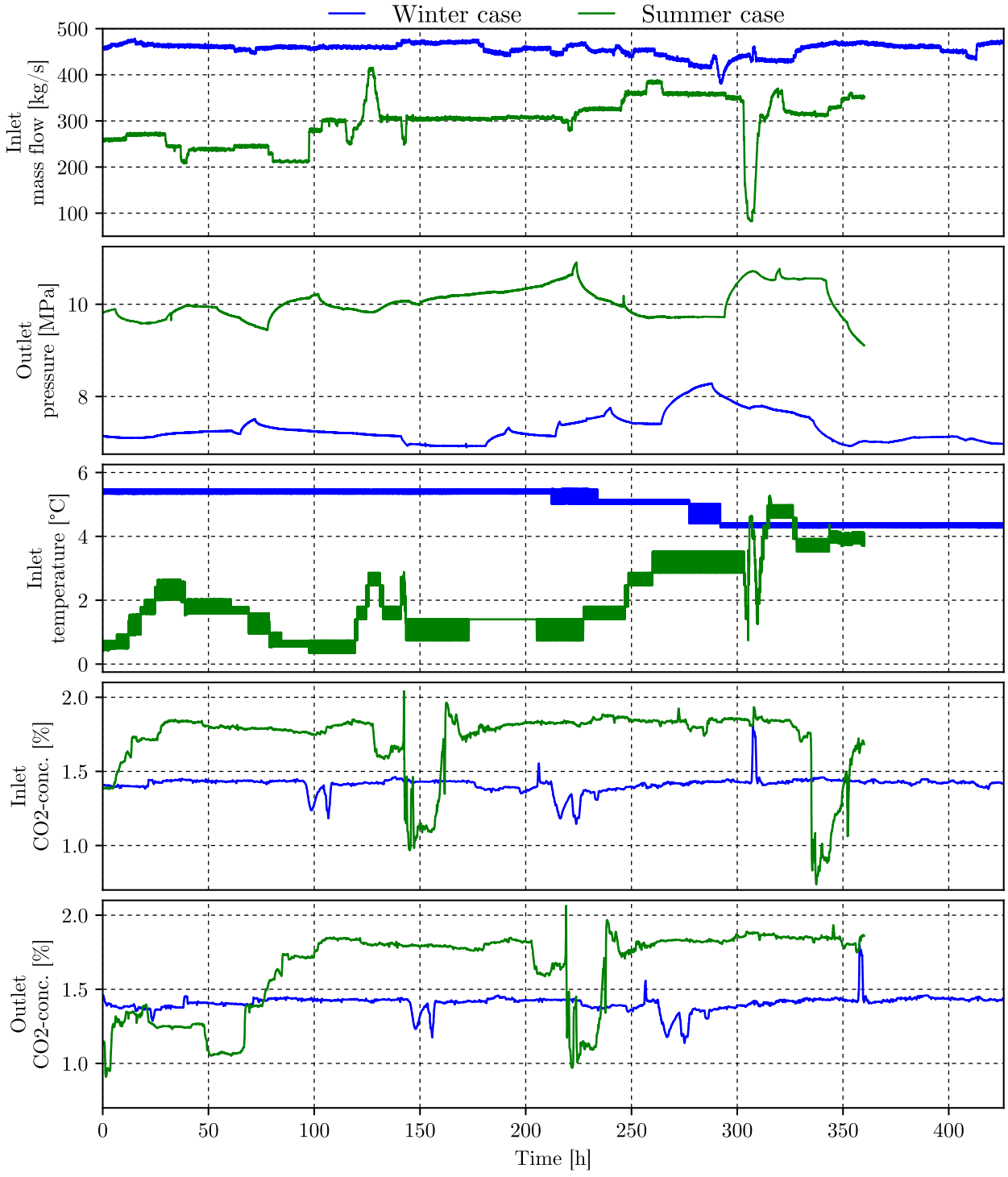


Figure 6: Boundary conditions used in the two simulation cases for the offshore pipeline; inlet mass flow, outlet pressure, inlet temperature and inlet CO2-concentration. The blue lines are 18 days from a winter period, and the green lines 14 days from a summer period. The flow rate is lower in the summer case than the winter case, which is typical for this pipeline, and is caused by lower demands for heating in the summer.

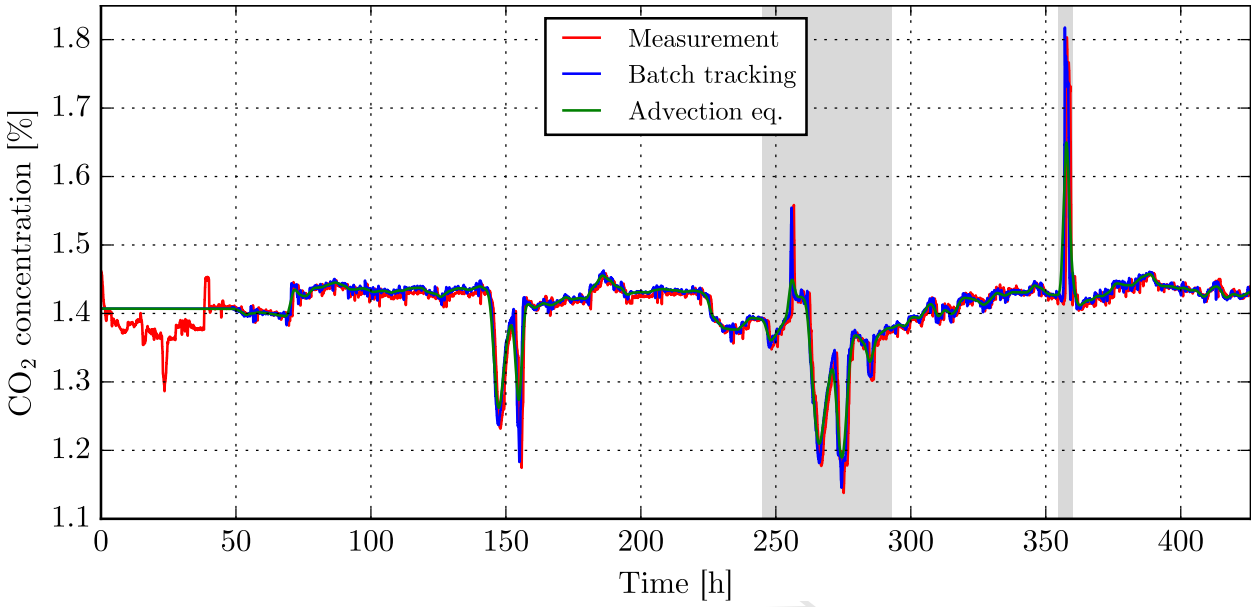


Figure 7: Plot of modeled and measured outlet $CO_2$-concentration for the winter case in the subsea pipeline. The gray shaded areas are shown in more detail in Fig. 8.

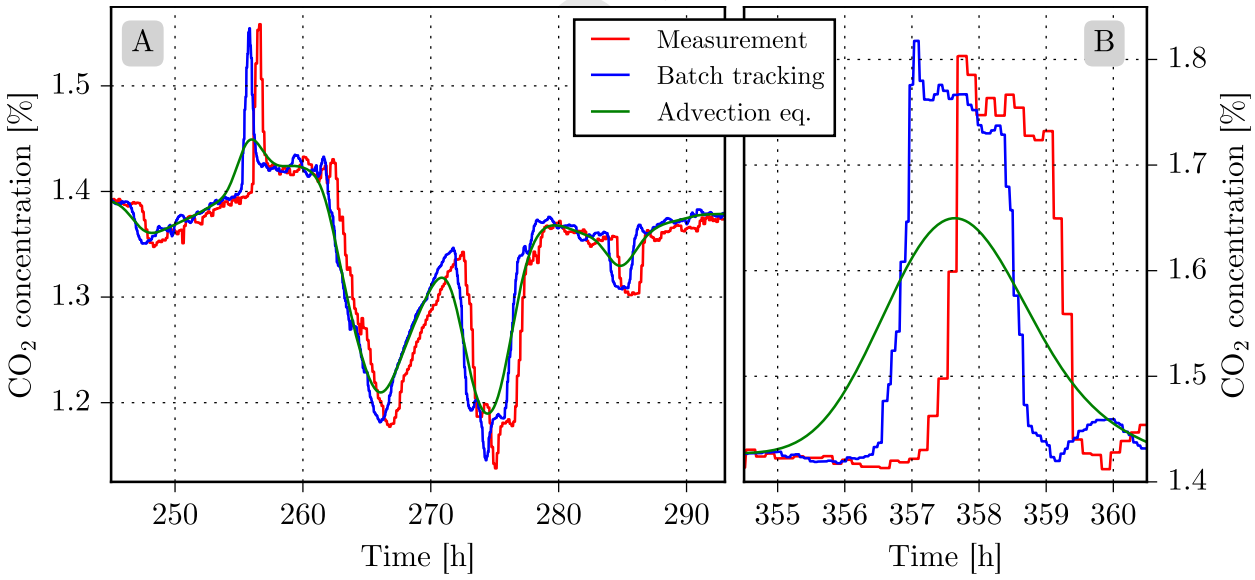


Figure 8: Details of the outlet $CO_2$-concentration for the winter case in the offshore pipeline shown in Fig. 7, showing (A) a 48-hour period between 245 hours and 293 hours (the widest of the two gray shaded sections in Fig. 7), and (B) a 6 hour period between 354.5 and 360.5 hours (the narrowest of the two gray shaded sections in Fig. 7).

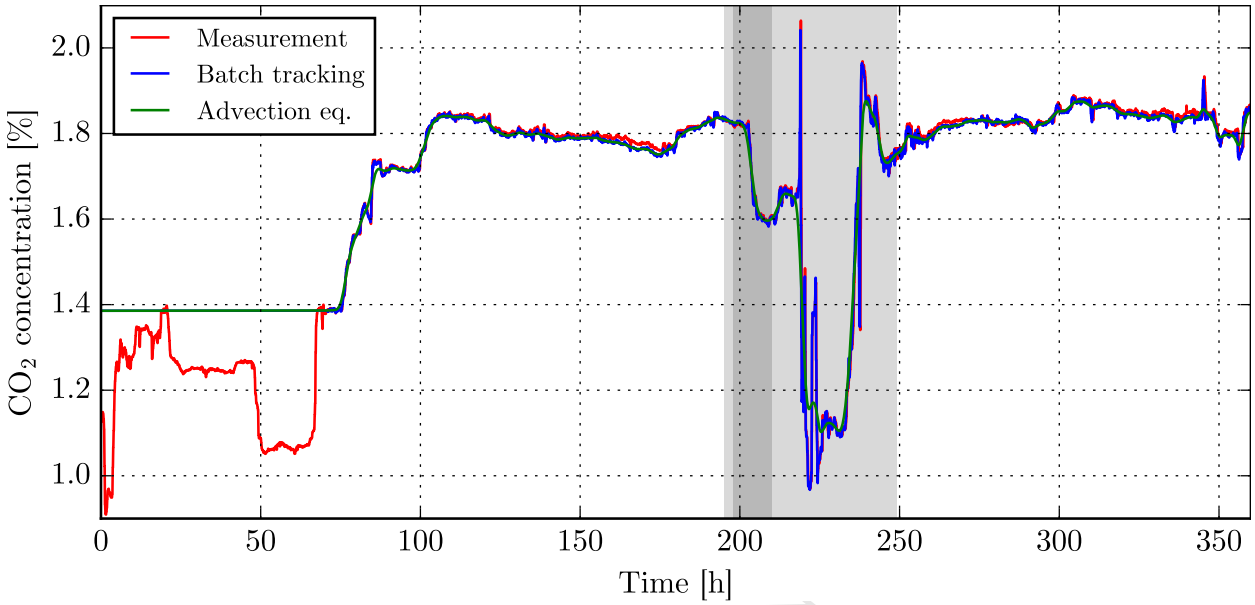


Figure 9: Plot of outlet $CO_2$-concentration for the summer case in the subsea pipeline. The gray shaded areas are shown in more detail in Fig. 10.

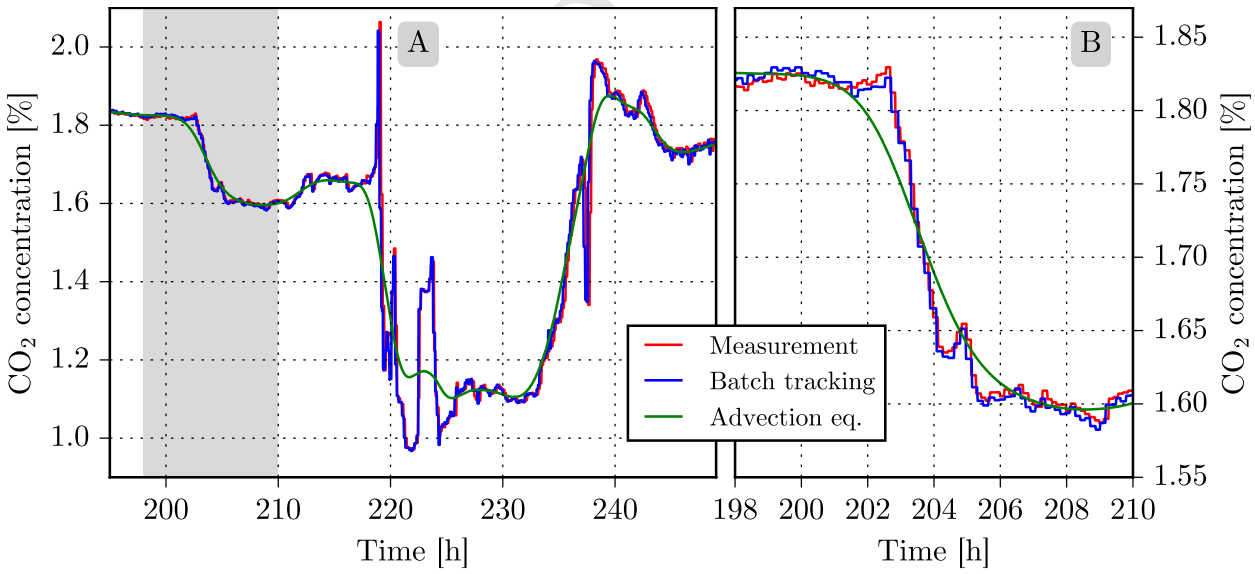


Figure 10: Details of the outlet $CO_2$-concentration for the summer case in the offshore pipeline shown in Fig. 9, showing (A) a 54-hour period between 195 hours and 249 hours (the widest of the two gray shaded sections in Fig. 9), and (B) a 12 hour period between 198 and 210 hours (the narrowest of the two gray shaded sections in Fig. 9).

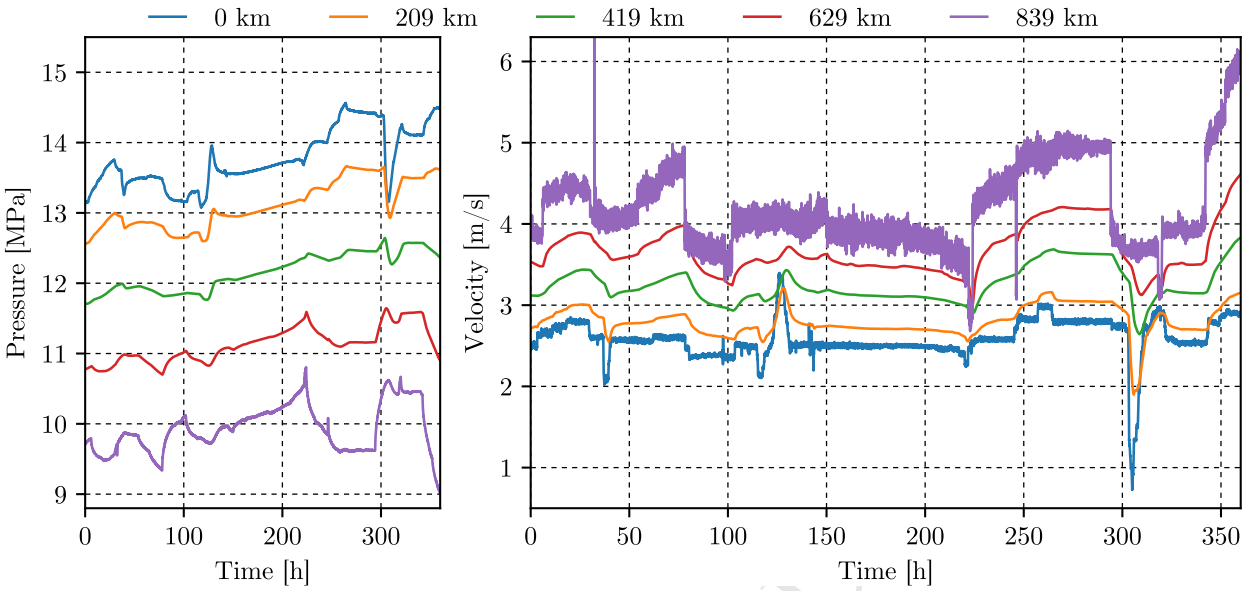


Figure 11: Plot of pressure and velocity evolution over time in the offshore pipeline during the summer case, for 5 selected locations along the pipeline (see the legend above the plots for the position of the selected locations).

## 6. Discussion

The results for the onshore pipeline presented in Fig. 4 and the offshore pipeline presented in Figs. 7 and 9 show that, on a daily scale, the transport times and concentrations predicted by both considered methods are quite similar, and in close agreement with the measurement data. Turning to the finer details shown in Figs. 5, 8 and 10, discrepancies in transport times of 10 to 25 minutes are observed for the onshore pipeline, and between 5 and 15 minutes for the offshore pipeline. The total transport time is around 23 hours for the onshore pipeline, and respectively 50 hours and 75 hours for the winter case and the summer case in the offshore pipeline. The relative errors in transport times are thus found to be up to 2 % of the total transport time.

The transport times predicted for the winter case in the offshore pipeline (Fig. 8) are constantly underestimated by around an hour. For the summer case and the onshore pipeline the error is smaller, with a tendency of underestimating the transport time, and it seems to be increasing slightly with time, especially for the batch tracking solution. These deviations for the onshore pipeline and for the summer case in the offshore pipeline can be attributed to the varying gas flow rates, whereas for the winter case in the offshore pipeline the gas flow rates are relatively invariant with time, as shown in the upper subplot of Fig. 6.

It can further be seen that the arrival time seems to be consistent between the two composition tracking methods, with the peaks and changes in concentration arriving at the outlet at approximately the same time. This indicates that the observed error in transport times is most likely due to errors in the modeled gas velocity, and not the methods themselves.

Careful observation of the results (Figs. 5, 8 and 10) shows that the concentrations

predicted by the implicit method have some discrepancies during periods with rapid changes, for both onshore and offshore pipelines. This can be attributed to the distortion in the predicted shape of the concentration profile, which is mainly caused by numerical diffusion of the finite difference scheme. Tests have shown that by using higher mesh densities, i.e. reducing $\Delta x$ and $\Delta t$ values, the effect of numerical diffusion on the solution can be reduced, but the drawback is an increased computation time. The batch tracking method largely eliminates the problem of numerical diffusion, and preserves both the linear-ramp and step profiles as they travel down the pipeline (see Fig. 8).

Table 1: Average error in modeled $CO_2$/ethane concentrations for the different cases and tracking methods. The initial periods with constant concentration present in the results are not included in the averages (the discarded periods are the first 22 h for the onshore pipeline, and respectively the first 50 h and 75 h for the winter and summer cases in the onshore pipeline).

| Case | | Tracking method | |
|---|---|---|---|
| | | Batch tracking | Implicit method |
| Offshore pipeline | Winter | 0.74 % | 0.66 % |
| | Summer | 0.55 % | 0.90 % |
| Onshore pipeline | | 0.86 % | 1.16 % |

The average error in modeled outlet concentration is calculated as

$$\frac{1}{n}\sum_{t=t_0}^{t_n}\frac{\left|c_{\text{modelled}}(t)-c_{\text{measured}}(t)\right|}{c_{\text{measured}}(t)},$$

where the sum is over all time steps in the simulations, disregarding the initial period $t_0$ before the pipeline is filled with gas with as-measured concentration. An overview of the average errors can be seen in Table 1. Both methods lead to comparable errors of around 1 % during typical pipeline operation. But it is also clear that the estimated error in modeled outlet concentration will depend a lot on the accuracy of the measurements of the concentration at both the inlet and the outlet. Additionally, the numerical diffusion observed with the implicit method will lead to a higher error during periods of large, rapid changes in concentration, but should in theory not affect the accuracy during periods with slower, smaller changes. Even though peak errors are larger when using the implicit method than batch tracking, as observed in Figs. 5, 8 and 10, these errors have little effect on the average error, since the average is taken over the whole time series.

Both gas composition tracking methods have low impact on computation time. As an example, in the case of the onshore pipeline, the difference in computation time for the fully implicit method with composition tracking compared to the fully implicit method *without* composition tracking was 31 %. The figures for batch tracking method were considerable lower. In the case of the onshore pipeline the difference was 22 %. The implicit method was computationally less efficient compared to its batch tracking counterpart, since it required the solution of a matrix equation at each time step. An increase of 22 % to 31 % is not unfeasible for applications of pipeline models.

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## 7. Conclusion

A gas composition tracking problem was solved combined with a detailed transport model (one dimensional non-isothermal flow model) to illustrate the operation of pipelines during transient flows with variable gas composition. Two approaches for tracking composition were presented, namely a fully implicit backward difference solution of the advection equation, and a batch tracking method. Some representative numerical examples for an onshore and an offshore pipeline were solved by the proposed approaches.

The results indicate that both methods are quite effective at finding transport times. The error in the predicted transport time for the 80 km-long onshore pipeline ranged from 0.7 % to 1.8 %, while the reported errors for the 800 km-long offshore pipeline were in the range from 0.1 % to 2.0 %. The errors in the predicted transport times were found to be sensitive to flow variations. The similarities between the errors in the transport times predicted by both methods indicate that the source for error is the gas velocity predicted by the flow model.

It was further found that the backward difference solution of the advection equation exhibits problems with numerical diffusion, smearing out small-scale structures in composition profile, especially in the presence of small bulk flow and sharp discontinuities. Conversely, the batch tracking method preserves the shapes of the composition profiles, without compromising the computational efficiency.

For decades, transmission systems comprised sources of supply based on long-term delivery contracts, therefore the quality of natural gas remained unchanged. Currently we no longer have such long-term physical stability in the systems, due to the fact that in many parts of the world new sources of gas are entering transmission system infrastructures. The situation has changed over the past few years and is continuing to change due to increased gas trading activities based on short-term contracts, substitution of pipeline-based by LNG-based supplies, and increasing injection of gases from non-conventional sources. There is also a broader interest in renewable gas injection into the grid (biomethane, hydrogen), which has begun to grow in recent years, especially in Europe, as a consequence of significant amount of power-to-gas research. The challenge of managing the diversification of gas quality can be accomplished using a modelling framework developed via the approach set out in this study.

## Acknowledgment

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- Two methods for tracking gas composition are applied and compared
- Estimated transport time errors below 2% for both on- and off-shore pipelines
- The moving grid method best preserves the details of changes in composition

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