Dynamic simulation of pipelines containing dense phase/supercritical CO₂-rich mixtures for carbon capture and storage

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Abstract
Carbon dioxide mixtures from separation plants contain usually some impurities. Major impurities include nitrogen, argon, hydrogen and oxygen, depending on the capture technology used for the removal of CO₂. The mixture composition determines the critical point data, and the values of critical pressure and critical temperature define, in turn, the limits of dense phase/supercritical pipeline operating conditions. The simulation of dynamic behaviour of three dense phase/supercritical CO₂-rich mixtures was carried out in this study. The pipeline CO₂ flow model was formulated with the assumption of one-dimensional, nonisothermal flow condition. An illustration of the performance of the model by an example of a fictive but realistic onshore CO₂ pipeline is given. The results show that the type and quantity of impurities have a significant influence on the hydraulics of the pipeline transportation system under transient conditions. They also indicate that the transportation costs vary and are dependent on the capture technology used.

Keywords: Carbon dioxide transport, Pipeline, Transient flow, CO₂-rich mixture, Dense phase CO₂, Supercritical CO₂

Nomenclature:

- \( A \) – area, \( m^2 \),
- \( c_p \) – specific heat at constant pressure, J/(kg K),
- \( D \) – pipe diameter, m,
- \( f \) – Darcy friction factor,
- \( g \) – the acceleration of gravity, m/s\(^2\),
- \( h \) – specific enthalpy, J/kg,
- \( k_L \) – linear heat transfer coefficient, W/(m K),
- \( m \) – element mass, kg,
- \( M \) – mass flow rate, kg/s,
- \( n \) – number of heat-transfer area discretization sections,
- \( N \) – number of pipeline discretization sections,
- \( p \) – gas pressure, Pa,
- \( q \) - rate of heat transfer per unit time and unit mass of the gas, W/kg,
- \( R \) – specific gas constant, J/(kg K),
- \( Re \) – Reynolds number,
- \( t \) – time, s,
- \( T \) – gas temperature, K,

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Alternative energies will play an increasingly important role in electricity generation, but the technology, infrastructure and regulatory framework for those energies are expected to take at least a decade or more to be deployed at scale. Viewed from this perspective, Carbon Capture and Storage (CCS) is considered as the path to cleaner, fossil fuel based energy sources. In the case of Poland it would allow coal to continue to play a major role in future energy mix. CCS, however, still faces a number of challenges, which include planning, design and operation of CO$_2$ transportation infrastructure.

Pipelines are the preferred mode of transportation for CO$_2$ when large volumes of captured CO$_2$ are to be stored in geological formations at short to medium distance from the capture location (Svensson et al., 2004). In the field of pipeline and compression facilities, the technical problems to be resolved involve pipeline integrity, flow assurance, safety and operational considerations. For a comprehensive review of the current development in CCS, see recently published review paper by Pires et al. (2011), while for commentary on the previous research work on CO$_2$ pipeline transportation, see the report by Oosterkamp and Ramsen (2008) and the paper by Vandeginste and Piessens (2008). It is beyond the scope of this article to make a detailed review of CO$_2$ transportation systems. Instead, the most recent research in the field of pipeline transportation with application to CCS will be mentioned briefly.

Carbon dioxide pipeline transport for enhanced oil recovery is a mature technology, however relatively little work has been carried out on CO$_2$ pipelines for CCS applications. Some research effort has been put in the area of steady-state flow modeling. Examples of such studies include those conducted by Zhang et al. (2006), McCoy and Rubin (2008), Seevam et al. (2008), Vandeginste and Piessens (2008) and, more recently, Nimtz et al. (2010).

Regarding the dynamics of CO$_2$ pipeline systems, there is very little work reported in the literature. Mahgerefteh et al. (2008) presented the results of the transient simulation of CO$_2$ pipeline rupture, obtained from the numerical solution of the conservation equations using the
method of characteristics. Peng-Robinson Equation of State (EOS) (Peng and Robinson, 1976) was used to describe the carbon dioxide properties. The comparison of the outflow data for the rupture of two identical pipelines each containing CO₂ and natural gas showed that the depressurization behavior of both pipelines was very similar, whereas the discharge rates maintained by the CO₂ pipeline were noticeably higher compared to those of the natural gas pipeline.

Munkejord et al. (2010) investigated the transport and depressurization parameters of a two-phase carbon dioxide-methane mixture using the Soave-Redlich-Kwong EOS (Soave, 1972). The multi-stage centered (MUSTA) scheme was employed for the numerical solution of the drift-flux model. The results indicated that mixture composition has an influence on mixture sonic speed and the cooling rate during depressurization.

Liljemark et al. (2011) evaluated the risk of phase transition during flow transients and pipe cooling of the transported CO₂/N₂ fluid mixture, consisting of 98% CO₂. Operation modes of load change, start-up, shut down and compressor trip were simulated using commercially available modeling environment. The Span and Wagner EOS (Span and Wagner, 1996) for carbon dioxide properties and GERG-2004 mixture model (Kunz et al., 2007) were used in the simulations.

In the study by Klinkby et al. (2011) the transient two-phase flow of carbon dioxide in the pipeline and well was investigated using a commercially-available multiphase flow simulator with Span and Wagner EOS. The modelling software package was shown to be a useful tool for integration of the transmission system and reservoir design activities, and allowed prediction of the phase conditions along the pipeline and in the well head.

Generally, there is an agreement that large volumes of CO₂ should be transported either as liquid or as a supercritical/dense phase fluid (Shafen and Carter, 2010). Dense phase is a preferable condition for transporting CO₂ in pipelines. This state is characterized by fluid viscosity similar to that of a gas, but a density closer to that of a liquid. Transmission in gaseous phase is not economical, as is the case with two-phase flow, in which high-pressure losses, particularly in hilly terrain, can occur.

The primary purpose of this work is to examine the hydraulic parameters of the CO₂ pipeline by solving the rigorous single-phase, compressible fluid flow model, suitable for supercritical and dense-phase CO₂ pipeline calculations, with relevance to CCS applications. The model is represented by one dimensional version of the Euler equations with source terms representing viscous dissipation of energy and heat transfer to the surroundings. Furthermore, it incorporates high precision reference equations of state explicit in the Helmholtz free energy from REFPROP 8.0 database (Lemmon et al., 2007) with GERG-2004 mixture model. The effect of different CO₂ mixture composition on flow properties in the pipeline is investigated. Finally, the energy demand for the compression processes is studied, which provides more insight into the operational costs of pipeline CO₂ transmission depending on the sequestration method in use.
2. Basic equations

2.1. Pipeline model

The basic equations are derived from the conservation principles. For one-dimensional, compressible fluid flow we have

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho w)}{\partial x} = 0 \]  
\[ \frac{\partial (\rho w)}{\partial t} + \frac{\partial \left( p + \rho w^2 \right)}{\partial x} = -f \rho w |w| - \rho g \sin \alpha \]  
\[ \frac{\partial}{\partial t} \left[ \left( u + \frac{w^2}{2} \right) \rho \right] + \frac{\partial}{\partial x} \left[ \left( h + \frac{w^2}{2} \right) \rho w \right] = \rho q - \rho wg \sin \alpha \]

where \( \rho \) is the density of the gas, \( w \) is the flow velocity, \( p \) is the gas pressure, \( f \) is the Darcy friction factor, \( D \) is the internal pipe diameter, \( g \) is the acceleration of gravity, \( \alpha \) is the angle between the direction \( x \) and the horizontal, \( u \) is the internal energy, \( h \) is the enthalpy of the gas, and \( q \) is the rate of heat transfer per unit time and unit mass of the gas. Eq. (2) can be converted using Eq. (1) to the following form

\[ dw + \frac{1}{\rho} \frac{\partial p}{\partial x} + f\rho w|w| + g \sin \alpha = 0 \]  

Substituting Eqs. (1) and (4) into the Eq. (3) and rearranging we obtain

\[ \rho \frac{\partial h}{\partial t} - \frac{\partial p}{\partial t} - \frac{f \rho w^3}{2D} = \rho q \]

Eqs. (1), (4) and (5) need to be rewritten with pressure, temperature and mass flow rate as the dependent variables, since the above parameters are typically measured and used in pipeline operations. Furthermore, we assume that the transmission pipeline will be operated with given CO₂ production rate and with the assumption of maintaining the storage site minimal delivery pressure. To obtain \( \rho \) and \( w \) in terms of \( p \), \( T \), and mass flow rate \( M \), we use the identity \( w = M \rho^{-1} A^{-1} \) and the relation for density \( \rho = \left( \frac{\partial p}{\partial T} \right)_p dT + \left( \frac{\partial \rho}{\partial p} \right)_T dp \) obtained from the appropriate EOS. The relationship for enthalpy is

\[ dh = c_p dT + \left[ 1 + \frac{T}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \right] \frac{dp}{\rho} \]

where \( c_p \) is the specific heat at constant pressure. The final form of continuity, momentum, and energy equations for one-dimensional pipeline flow is

\[ E(p,T) \frac{\partial p}{\partial t} + F(p,T) \frac{\partial T}{\partial t} = G(p,T) \]

\[ H(p,T) \frac{\partial M}{\partial t} = I(p,T) \]

\[ J(p,T) \frac{\partial p}{\partial t} + K(p,T) \frac{\partial T}{\partial t} = N(p,T) \]

where: \( E(p,T) = \left( \frac{\partial \rho}{\partial p} \right)_T \), \( F(p,T) = \left( \frac{\partial \rho}{\partial T} \right)_p \), \( G(p,T) = -\frac{1}{A} \frac{\partial M}{\partial x} \), \( H(p,T) = \frac{1}{A} \).
\[ I(p,T) = \left( \frac{M}{\rho A} \right)^2 \left( \frac{\partial \rho}{\partial p} \right) \left( \frac{\partial p}{\partial T} \right)^{-1} \frac{\partial T}{\partial x} - \frac{2M}{\rho A^2} \frac{\partial M}{\partial x} + \left( \frac{M}{\rho A} \right)^2 \left( \frac{\partial \rho}{\partial T} \right) \left( \frac{\partial T}{\partial p} \right) - \frac{2fM|M|}{D\rho A^2} - \rho g \sin \alpha \]

\[ J(p,T) = \frac{T}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \cdot K(p,T) = \rho c_{p, r}, N(p,T) = \frac{MT}{\rho A} \left( \frac{\partial \rho}{\partial T} \right)_p \frac{\partial p}{\partial A} - \frac{c_{M} M \partial T}{A \partial x} + \frac{2fM^3}{D\rho A^3} - \frac{k_0}{A} (T - T_i) \]

where \( A \) is the pipeline cross-section area, and \( k_0 \) denotes heat transfer coefficient between the gas and the first element. Eqs. (7), (8) and (9) constitute the set of nonlinear partial differential equations (PDE) of hyperbolic type governing one-dimensional flow of compressible fluid. For closure of the above set of equations, an equation of state must be used. In this study, the calculation of density and its derivatives with respect to pressure and temperature has been performed using GERG-2004 mixture model and the pure substance equations of state listed in Table 1.

### Table 1. Composition (mole fractions) of CO\(_2\) mixtures from different capture technologies with estimated critical properties

<table>
<thead>
<tr>
<th>Pure CO(_2)</th>
<th>Post-combustion</th>
<th>Pre-combustion</th>
<th>Oxyfuel</th>
<th>EOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide</td>
<td>1.000</td>
<td>0.998</td>
<td>0.970</td>
<td>0.857</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.002</td>
<td>0.030</td>
<td></td>
<td>0.066</td>
</tr>
<tr>
<td>Hydrogen</td>
<td></td>
<td></td>
<td>0.029</td>
<td></td>
</tr>
<tr>
<td>Oxygen</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Argon</td>
<td></td>
<td></td>
<td>0.048</td>
<td></td>
</tr>
<tr>
<td>critical pressure (MPa)</td>
<td>7.3773</td>
<td>7.3515</td>
<td>7.0075</td>
<td>8.5232</td>
</tr>
<tr>
<td>critical temperature (K)</td>
<td>304.13</td>
<td>303.59</td>
<td>296.00</td>
<td>288.36</td>
</tr>
</tbody>
</table>

The process of heat transfer from the gas to the surroundings of the pipeline has been described using unsteady heat transfer model, so that the effect of heat capacity of the surroundings of a pipeline could be taken into consideration. An axisymmetric heat transfer model has been adopted, and the surroundings of the pipeline were modelled by four coaxial cylindrical layers as heat capacitors.

\[
\frac{m_i c_{pi}}{dx} \frac{\partial T_i}{\partial t} = k_i (T_i - T_1) - k_{i-1} (T_{i-1} - T_i) \tag{10}
\]

\[
\frac{m_i c_{pi}}{dx} \frac{\partial T_2}{\partial t} = k_i (T_i - T_2) - k_2 (T_2 - T_3) \tag{11}
\]

\[
: \frac{m_i c_{pi}}{dx} \frac{\partial T_n}{\partial t} = k_{n-1} (T_{n-1} - T_n) - k_n (T_n - T_{ground}) \tag{12}
\]

where \( n \) is the number of discretization sections of heat-transfer area (equal to number of elements), \( m_i \) is element mass \((i = 1, \ldots, n)\), \( c_{pi} \) is the specific heat of element \( i \), \( m_i c_{pi} \) is the element heat capacity per pipeline unit length, \( dx \) is the discretization section of a pipeline, \( T_i \) is the element temperature, and \( k_i \) is the heat transfer coefficient between elements \((i-1)\) and \( i \).

Eqs. (10)-(12) are the heat balance equations of the coaxial cylindrical layers representing the heat-transfer model of the surroundings of the pipeline. An assumption was made in this study.
that for every discretization section of the pipeline there are four such layers \((n = 4)\), serving as heat capacitors, with the temperature \(T_1\) through \(T_4\), while the temperature \(T\) at the internal radius of the first layer is the gas temperature, and the temperature \(T_{ground}\) at the external radius of the last layer is the surface air temperature. The three governing equations for gas pressure, temperature and mass flow-rate were coupled with four heat balance equations and solved simultaneously as one system of PDEs.

The initial values for the partial differential equations were obtained by setting the time derivatives in Eqs. (1)–(3) equal to zero, and solving the resulting set of ordinary differential equations.

\[
\begin{align*}
\frac{dp}{dx} &= (SV - BZ)(PV - QU)^{-1} \\
\frac{dT}{dx} &= (PZ - SU)(PV - QU)^{-1}
\end{align*}
\] (13)

where coefficients \(P, Q, S, U, V, Z\) are known functions of temperature and pressure:

\[
P = \frac{1}{\rho} \left(\frac{M}{A}\right)^2 \frac{1}{\rho^1} \left(\frac{\partial \rho}{\partial p}\right)T, \quad Q = -\left(\frac{M}{A}\right) \frac{1}{\rho^3} \left(\frac{\partial \rho}{\partial p}\right)T, \quad S = -\frac{f}{2D} \left(\frac{M}{\rho A}\right)^2 - g \sin \alpha, \quad U = \frac{T}{\rho^2} \left(\frac{\partial \rho}{\partial T}\right)_p, \quad V = c_p,
\]

\[
Z = \frac{f}{2D} \left(\frac{M}{\rho A}\right)^2 - \frac{k_L}{M} (T - T_{ground}), \quad \text{and} \quad k_L \text{ is the overall linear heat-transfer coefficient.}
\]

The values of \(\rho, (\partial \rho / \partial p)_T \text{ and } (\partial \rho / \partial T)_p\) are determined from the equation of state.

The overall linear heat-transfer coefficient for onshore pipelines is calculated from the expression:

\[
k_L = \left(\frac{1}{\pi D h_{conv}} + \sum_{i=1}^{m} \frac{1}{2\pi \lambda_i} \ln \left(\frac{D_i}{D_{i-1}}\right) + R_{ground}\right)^{-1}
\] (15)

where \(h_{conv}\) is the convection heat transfer coefficient, \(\lambda_i\) is the thermal conductivity of the \(i\)-th pipe wall layer, and \(R_{ground}\) is the thermal resistance of the ground. Eq. (15) shows that the overall heat transfer resistance is equal to the sum of three individual resistances resulting from the convection between the gas and the inner pipe wall, the conduction in the pipe wall, and the conduction in the ground. It can be shown, that the surface resistance on the inner pipe wall, and the conduction resistance of the pipe wall are less than 1% of the total heat transfer resistance (Gersten et al., 2001). Therefore, it is sufficient to consider the heat transfer within the ground only. A well-known analytical solution for heat conduction problem between the pipe with depth \(H\) below the ground surface and the surroundings of the pipe (semi-infinite solid) leads to the following formula for the ground resistance

\[
R_{ground} = \frac{1}{2\pi \lambda_{ground}} \ln \left(\frac{H}{D} + \left(\frac{H}{D}\right)^2 - 1\right)
\] (16)

where \(\lambda_{ground}\) is the thermal conductivity of the ground, and \(D\) is the pipe outside diameter. For the purpose of heat-transfer area discretization, the assumption was made that every cylindrical element \((i = 1, \ldots n)\) has the same thermal resistivity, i.e. \(k_0 = k_n = \left(\frac{R_{ground}}{l(2n)}\right)^{-1}\), \(k_i = \left(\frac{R_{ground}}{n}\right)^{-1}, \quad i = 1, \ldots n - 1\), thus the temperature differences between consecutive ground
sections under steady-state conditions were equal, and the initial condition could be accurately modelled. The equations (13) and (14) are solved in this study using the fourth order Runge–Kutta method for the initial values of pressure and temperature in the pipeline.

2.2. Compressor model

The required work input to a compressor for a defined control period is obtained from the following equation

$$W_{\text{comp}} = \int_0^t \dot{W}_{\text{comp},i} \cdot \mathrm{d}t$$

(17)

The sum of power input to all stages of compression is determined form

$$\dot{W}_{\text{comp},i} = \sum_i M \cdot (h_d - h_i)$$

(18)

The exit enthalpy of the $i$-th stage is calculated using isentropic efficiency of the compressor

$$h_i = h_i + (h_{i,d} - h_i) / \eta_{\text{comp}}$$

(19)

The exit enthalpy for the isentropic process is determined from flash calculation given pressure and entropy $h_{i,d} = h(s_d, p_d)$, while the exit entropy is calculated from the requirement that the entropy of the gas remains constant ($s_d = s_i$), i.e. $s_d = s(p_i, T_i)$. The exit temperature of the $i$-th stage is determined from the flash calculation given pressure and enthalpy $T_d = T(p_d, h_d)$.

3. Solution method

Method of lines (MOL) was selected for the numerical solution of the system of the conservation equations. MOL proceeds with two separate steps: (1) spatial derivatives approximation, and (2) time integration of the resulting ordinary differential equations (ODE). In this study finite difference scheme with two techniques for spatial discretization is used, namely the fixed-grid method and the moving grid method, in the solution of slow transient and fast transient processes, respectively.

The system of PDEs was converted to the following system of discrete in space and continuous in time ODEs, by solving the Eqs. (7), (8) and (9) for the derivatives of pressure, flow rate and temperature

$$\frac{\partial p}{\partial t} = \frac{F(p_j, T_j)N(p_j, T_j) - G(p_j, T_j)K(p_j, T_j)}{F(p_j, T_j)J(p_j, T_j) - E(p_j, T_j)K(p_j, T_j)}, \quad j = 0,1,\ldots,N$$

(20)

$$\frac{\partial M}{\partial t} = \frac{H(p_j, T_j)}{I(p_j, T_j)}, \quad j = 0,1,\ldots,N$$

(21)

$$\frac{\partial T}{\partial t} = \frac{G(p_j, T_j)J(p_j, T_j) - E(p_j, T_j)N(p_j, T_j)}{F(p_j, T_j)J(p_j, T_j) - E(p_j, T_j)K(p_j, T_j)}, \quad j = 0,1,\ldots,N$$

(22)

where: $G(p_j, T_j) = -\frac{1}{A} \Delta x \left( M_j \right)$. 

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\[ I(p_j, T_j) = -\frac{M_j \rho_j}{\rho_j A^2} \Delta x \left( M_j \right) + \left[ \frac{M_j}{\rho_j A^2} \left( \frac{\partial \rho}{\partial p} \right)_{T_j} - 1 \right] \Delta x \left( p_j \right) \]
\[
+ \left( \frac{M_j}{\rho_j A^2} \right)^2 \left( \frac{\partial \rho}{\partial p} \right)_{T_j} \Delta x \left( T_j \right) - 2fM_j \frac{M_j}{\rho_j A^2} - \rho_j g \sin \alpha, \]
\[ J(p, T) = \frac{T_j}{\rho_j} \left( \frac{\partial \rho}{\partial T} \right)_{T_j}, \quad K(p, T) = \rho_j c_{p,j}, \]
\[ N(p, T) = -\frac{M_j}{\rho_j A} \left( \frac{\partial \rho}{\partial T} \right)_{T_j} \Delta x \left( p_j \right) - \frac{c_p M_j}{A} \Delta x \left( T_j \right) + \frac{2fM_j}{D \rho_j A^4} - \frac{k_0}{A} \left( T_j - T_i \right) \]

and \( j \) is the spatial coordinate discretization section index, \( N \) is the number of pipeline discretization sections, \( \frac{\partial p_j}{\partial x} \equiv \Delta x \left( p_j \right) \), \( \frac{\partial M_j}{\partial x} \equiv \Delta x \left( M_j \right) \) and \( \frac{\partial T_j}{\partial x} \equiv \Delta x \left( T_j \right) \) are the algebraic formulas for the approximation of spatial derivatives.

The governing equations for gas pressure, temperature and mass flow rate are coupled with the heat balance equations of the coaxial cylindrical layers representing the heat transfer model of the surroundings of the pipeline, and solved simultaneously as one system of PDEs in each time step.

3.1. Fixed-grid spatial differentiation
In the test case of a slow transient processes in the CO2 transmission pipeline, the three-point differentiation formula for spatial derivatives approximation was adopted (Carver and Hinds, 1978). As an example, the differentiation matrix for spatial derivative of pressure is

\[
\begin{bmatrix}
\frac{\partial p(x_0)}{\partial x} \\
\frac{\partial p(x_1)}{\partial x} \\
\vdots \\
\frac{\partial p(x_{N-1})}{\partial x} \\
\frac{\partial p(x_N)}{\partial x}
\end{bmatrix}
\equiv \Delta_X (p) = \frac{1}{2\Delta x}
\begin{bmatrix}
-3 & 4 & -1 & 0 & \cdots & 0 & p(x_0) \\
-1 & 0 & 1 & 0 & \cdots & 0 & p(x_1) \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & -1 & 0 & 1 & p(x_{N-1}) \\
0 & \cdots & 0 & 1 & -4 & 3 & p(x_N)
\end{bmatrix}
\] (23)

Above approximation is second-order correct, i.e. the truncation error is proportional to \( \Delta x^2 \). The differentiation matrix (23) results from the second-order central finite difference approximation for the first derivative of the dependent variable \( du(x_i)/dx \).

3.2. Moving-grid method
The computational stencil (23) can produce spurious numerical oscillations in the solution of the problem developing steep spatial moving fronts (Schiesser, 1991). In the first test case considered in this study, severe transient conditions were created by the downstream valve closure. To avoid undesirable oscillations in the solution profiles, a moving grid algorithm implemented by Blom and Zegeling (1994) for the adaptation of the spatial grid is used. The grid consists of moving grid nodes \( X_j(t), j = 1, N-1 \) for the inner spatial domain (time-dependent grid points) and fix grid nodes at the domain boundaries \( X_0 \) and \( X_N \), respectively.

Generally, the system of PDEs (20)-(22) coupled with heat-transfer equations (10)-(12) is in the form
\[ \frac{\partial \mathbf{u}}{\partial t} = \mathbf{F}(u,x,t) \]  

(24)

where \( \mathbf{u} = [p \ M \ T \ T_1 \ T_2 \ ... \ T_n]^T \) and \( \mathbf{F} \) is the vector with right-hand-sides of the respective equations. The above system of \( n + 3 \) component PDEs is transformed to its Lagrangian form, using the total differential

\[ \frac{d\mathbf{u}}{dt} - \mathbf{D} \frac{d\mathbf{X}}{dt} = \mathbf{F}(u,X,t) \]  

(25)

Where \( \mathbf{D} = \begin{bmatrix} u_{j+1} - u_j \\ X_{j+1} - X_j \end{bmatrix} \), \( 1 \leq j \leq N - 1 \) is the solution dependent matrix representing second order discretisation in space to the exact PDE solution \( \mathbf{u} \), and \( \mathbf{F} \) is the vector with right-hand-side function of PDEs at the point \((X(t), t)\).

The general form of the moving grid equations reads

\[ \tau \mathbf{B} \frac{d\mathbf{X}}{dt} = \mathbf{G}(u,X,\kappa) \]  

(26)

where the positive parameter \( \tau \) is acting as a time-constant preventing sudden changes in the grid movement and avoiding temporal oscillation of the grid, the matrix \( \mathbf{B} \) as well as the function vector \( \mathbf{G} \) are derived so as to equally distribute a monitor function \( m(u,x) \) considering the spatial gradients of the solution

\[ m(u,x) = \sqrt{\alpha + \frac{1}{n+3} \sum_{i=1}^{n+3} \left( u_{j+1} - u_j \right)^2 / (\Delta X_j)^2} \]  

(27)

In order to avoid excessive spatial distortion, a regularization procedure, namely spatial smoothing technique, is used. A positive parameter \( \kappa \), such that

\[ \frac{1}{1+\frac{1}{\kappa}} \leq \frac{X_{j+1} - X_j}{X_{j+1} - X_j} \leq 1 + \frac{1}{\kappa} \]  

(28)

is used to control the grid expansion. Above property provides “local quasi-uniformity” and means that the variation in successive grid cells can be controlled at every point in time. A more detailed discussion of this smoothing technique can be found in Verwer et al. (1989).

Eqs (24) and (26) are combined to yield the system of stiff DAEs, which can be solved with a variable step integrator.

### 3.3. Time integration

The DASSL solver (Petzold, 1983), which is a variable stepsize variable order integrator, is used in this study for time integration of the system of stiff DAEs. On every step it chooses the order (ranges from one to five) and stepsize based on the behavior of the solution. DASSL decides what stepsize to use on the next step after the order of the method to be used on the next step has been determined. The new stepsize is chosen so that the error estimate satisfies both the local truncation error and the interpolation error due to interpolating the true solution by a polynomial. The error at the new order \( k \) is estimated as if the last \( k + 1 \) steps were taken at the new stepsize, and the new stepsize is chosen so that the error estimate satisfies the requested integration error tolerance. More precisely, DASSL chooses the new step size so that the error reflected in the weighted norm of the predictor-corrector difference is roughly one half of the desired integration error tolerance. After a successful step, the stepsize is increased only if it can be doubled. The stepsize is reduced by a factor at least 0.9 and at most 0.25. The detailed description of DASSL code can be found in Brenan et al. (1996).
4. Case study

In this section, we give numerical results representative for an ongoing CCS project in Belchatów power plant, which was accepted together with six other European projects for a programme implemented within the framework of the European Energy Programme for Recovery (EEPR) initiative. Located in central Poland, the plant is the Europe's largest lignite-fired power plant by capacity. It has been selected by the European Union to implement a demonstration CCS project on approximately 260 MW. The plant will capture carbon dioxide coming from the 33% of the flue gas stream leaving the 858 MW supercritical power generation unit, currently under construction. The operation of a full-scale 858 MW demonstration plant is scheduled for 2015. The compressed gas will be transported to underground saline aquifer. Three different saline aquifer sites, located approximately 61 km, 72 km and 140 km away from the capture plant are to be investigated in this project. The site located 140 km away from the capture plant was selected for the analysis in this study (Figure 1). The post-combustion capture technology is to be chosen, and with the expected capture rate in excess of 80% it should allow for the separation of 2.1 million tonnes of CO₂ per year. For the case studies under consideration, the average steady state flow rate was estimated to be 70 kg/s.

Taking into account the possibility of different capture technologies to be employed over the lifetime of the power plant, the CO₂ streams with different combination of impurities, corresponding to the three capture technologies, namely: Post-combustion, Pre-combustion, and Oxyfuel were considered for the purpose of the hydraulic analysis of the CO₂ transmission system in this study. The Post-combustion and Pre-combustion processes were modelled by binary combinations of CO₂ with nitrogen and hydrogen, respectively, while Oxyfuel technology was represented by a four component mixture of CO₂, nitrogen, oxygen, and argon. The detailed composition of the CO₂ streams is presented in Table 1. The amounts of impurities are the normalised values obtained from their relative percentage in the CO₂ mixtures, based on potential impurity limits presented by Oosterkamp and Ramsen (2008). It has been assumed that in the case of Pre-combustion and Oxyfuel technologies, the concentrations of H₂S and SO₂ will be much lower than the figures for impurities presented in Table 1, and small enough to be neglected. The critical temperature and pressure values of the CO₂ streams in Table 1 were obtained from REFPROP 8.0 database which was also used for the calculation of density and its derivatives in the pipeline model. It should be noted that the number of impurities in the captured CO₂ streams can be greater than those presented in Table 1, however, the literature survey conducted by Oosterkamp and Ramsen (2008) shows that the expected fractions of the remaining impurities should be at least one order of magnitude lower than figures listed in Table 1. In case of Pre-combustion and Oxyfuel mixtures, more impurities could not be included in the analysis with the use of REFPROP 8.0 database anyway, since it reports no reliable mixing parameters for mixtures containing hydrogen and sulphur dioxide in combinations with given Pre-combustion and Oxyfuel mixture components.

Two case studies, describing the block valve closure scenario, and the effect of load change in the transmission pipeline are investigated to provide a better understanding of thermal and hydraulic processes during the CO₂ transport. Before going over to analysis of unsteady flow conditions in the entire pipeline, the simple case of a fast transient in a pipeline section will be considered.
4.1. Block valve closure

First test was carried out to present the effect of CO$_2$ mixture composition on the pipeline hydraulics during block valve activation downstream of the compressor station (Fig. 1). Let us suppose a line section of 10 km in length with no elevation changes, 406.4 mm outside diameter with a wall thickness of 12.7 mm, transporting a CO$_2$ mixture at a pressure of 9.5 MPa and a temperature of 40ºC to ensure that the CO$_2$-impurity combination was in the dense phase. Now the block valve closes, and the outflow drops down from 70 kg/s to zero over a period of 60 s, while the inlet pressure is held at 9.5 MPa. After maintaining this condition for 20 minutes, the block valve is opened to allow full flow rate to be re-established within a period of 60 s. The roughness of 0.046 mm, typical for commercial steel pipe, is assumed, and the Darcy friction factor is obtained from the iterative solution of the Colebrook – White equation (Colebrook, 1939) using Newton's method

\[
\frac{1}{\sqrt{f}} = -2.0\log \left( \frac{\varepsilon}{3.7D} + \frac{2.51}{Re\sqrt{f}} \right)
\]

(29)

In case of CO$_2$ fluid, the viscosity in the Reynolds number parameter was determined from the model by Fenghour et al. (1998), while for the CO$_2$ mixtures with impurities, the values of viscosity were obtained from an extended corresponding states method by Klein et al. (1997).

The properties of the pipeline burial depth of 1.5 m is assumed, and the ground temperature is assumed to be 5ºC.

![Fig. 1. Structure of the CO$_2$ pipeline in case study 1, CS-compressor station, BV-block valve.](http://repo.pw.edu.pl)

Table 2. Properties of pipe wall and the surrounding soil

<table>
<thead>
<tr>
<th>Pipe wall structure</th>
<th>Thickness (mm)</th>
<th>$\lambda$ (W/m·K)</th>
<th>$\rho$ (kg/m$^3$)</th>
<th>$c_p$ (J/kg K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel API 5L X-70</td>
<td>12.7</td>
<td>45.3</td>
<td>7830</td>
<td>500</td>
</tr>
<tr>
<td>External coating (polyethylene)</td>
<td>3.0</td>
<td>0.4</td>
<td>940</td>
<td>1900</td>
</tr>
<tr>
<td>Soil</td>
<td>1500</td>
<td>1.0</td>
<td>1640</td>
<td>1530</td>
</tr>
</tbody>
</table>

The results of the numerical experiment aiming at studying the effect of the grid refinement are presented in Figs. 2 and 3, taking CO$_2$ fluid as an example. Fig 2. shows comparison between different spatial discretization stages ($N = 5, 10, 50$ and $100$) for the inlet flow rate, while Fig 3. shows comparison for the outlet pressure. It can be observed that ten sections of the pipe and four elements of the heat-transfer area in the surroundings of the pipeline were found to be a sufficient discretization stage for this particular problem. For the validation of the adaptive grid MOL, the pressure wave and the flow rate wave propagation at the time of
the valve closure was investigated, taking again CO\(_2\) fluid as an example, and the results are presented in Figs. 4 and 5. Multiple lanes show the pressure and flow rate waves while travelling backwards along the pipeline during the valve closure. The time interval between two consecutive wave fronts is 10s. The numerical results show, that the proposed methodology can be considered as appropriate for the predictions of fast transient processes in the CO\(_2\) pipeline, since no numerical oscillations are present in the moving grid solutions. Figures 6 and 7 show the pressure and temperature variation with time at the block valve station. The maximum pressure ranged from 9.559 MPa and 9.565 MPa, respectively, for the Oxyfuel and Pre-combustion mixtures, to 9.599 MPa and 9.595 MPa for CO\(_2\) and Post-combustion mixture. The largest pressure and temperature drop corresponds to Oxyfuel stream, followed then by Pre-combustion and Post-combustion streams, which confirms previous results by Seevam et al (2008) for the steady-state conditions. The results show that viscous resistance of the CO\(_2\)/N\(_2\) mixture representative for the Post-combustion process is very similar to that of a CO\(_2\) stream due to low impurity concentration.

![Fig. 2. Effect of spatial grid refinement on the inlet mass flow rate in the pipeline, a) overall operating conditions, b) valve opening conditions, c) valve closure conditions.](image-url)
Fig. 3. Effect of spatial grid refinement on the outlet pressure in the pipeline, a) overall operating conditions, b) valve closure conditions, c) valve opening conditions.

Fig. 4. Pressure wave propagation during block valve closure.
The valve closure causes the fluid to decelerate, and the pressure at the block valve station to increase, whereupon it starts to oscillate around the final value of 9.5 MPa. Eventually this oscillation is damped out due to frictional energy dissipation. The maximum amplitude of the pressure waves was 0.014 MPa with a period of 165 s. for the Post-combustion stream, and with a period of 180 s. for the Pre-combustion stream. Similar results were seen for Oxyfuel mixture, which showed the same period of 180 s., however slightly lower value of 0.12 MPa with regard to maximum amplitude was observed. The CO$_2$ fluid also showed the amplitude of 0.012 MPa, but the period was 135 s.

Sudden compression and expansion resulting from the block valve closure and reopening causes the largest temperature change in CO$_2$ stream from Oxyfuel source. Figure 7 also demonstrates that the Oxyfuel mixture shows the fastest cooling rate during the simulated transmission stop. Cooling of the gas in the pipeline occurs (for example at $t = 20$ min. and thereafter) due to the heat transfer with the surroundings of the pipeline.
The effect of impurities in CO₂ stream on the mass flow rate at the compressor station is shown in Figure 8. The presence of impurities affects the flow-rate necessary to maintain a constant discharge pressure at the compressor station. The mass flow rate at the time of the valve reopening drops down to 6.68 kg/s in case of Oxyfuel mixture, while for the Post-combustion and Pre-combustion mixtures the figures where 7.00 kg/s and 8.07 kg/s, respectively. This compares to 6.82 kg/s of the CO₂ stream. The oscillations in the flow rate are symmetrical about the above values. The relatively small and positive value of the flow rate at the pipeline inlet after the valve closure is caused by the assumed left boundary condition, i.e. small amounts of gas need to be delivered to the pipeline in order to maintain the constant pressure at the pipeline inlet.

![Fig. 8. Variation of mass flow rate at the compressor station.](image)

The oscillations in the flow rate are gradually damped out by viscous dissipation. The mass flow rate was found to oscillate with the maximum amplitude of 9.9 kg/s and 9.6 kg/s for CO₂ and Post-combustion streams, respectively. The corresponding amplitude value for both Pre-combustion and Oxy-fuel streams was 9.6 kg/s. The flow rate oscillation period for CO₂ and Post-combustion streams was 240 s. against 285 s. of Pre-combustion stream and 255 s. of Oxyfuel stream.

In summary, the simulation results presented in Figures 6 through 8 show that the computed flow of CO₂ mixtures behaves differently at different time steps during the sudden flow change like valve open/close event discussed in this scenario.

### 4.2. Variable CO₂ production rates

In this test, variable CO₂ production rates were simulated, assuming that the mass flow rate in the capture plant varies linearly at a rate of 0.25 kg/min between the values of 40 and 100 kg/s as demonstrated in Fig. 9. The transmission pipeline with the same diameter, but a length of 140 km (Fig. 10) was used to explore the influence of impurities on the operating conditions, over a 24h control period. The length of the pipeline corresponds with the distance to one of the possible saline aquifer sites to be investigated under Belchatów CCS project. Ten kilometre long discretization sections were sufficiently small for this particular problem.

According to Nimtz et al. (2010), the CO₂ pressure should be at least 10 bar above the critical pressure to ensure that the supercritical conditions are maintained regardless of the flow conditions. Therefore, the constant delivery pressure, equal to 10 bar above the critical pressure of the respective CO₂ mixture (Table 1), was set as the boundary condition at the end of the pipeline (delivery node), except for oxyfuel mixture, for which the delivery pressure of 20 bar above the critical pressure was necessary to avoid two-phase flow conditions in the pipeline (Fig. 11). These assumptions are applicable only under the condition that the
minimum suction pressures necessary to compress the CO\textsubscript{2} mixtures in compressor station CS2 (Fig. 10) are lower than the above mentioned values.

![Fig. 9. Variation of mass flow rate at the compressor station (boundary condition).](image)

![Fig. 10. Structure of the CO\textsubscript{2} transmission system, CS1-compressor station in capture and separation plant (sending node), CS2-compressor station in storage plant, DN-delivery node in injection plant, IW-injection well.](image)

The generic model of a 4-stage reciprocating compressor as described in section 2.2 was solved in order to estimate the compression power necessary to transport the CO\textsubscript{2} mixtures considered in this study. It has been assumed that the compressor incorporated three intercoolers, in which the gas was cooled to 40ºC, while the maximum discharge temperatures were set to 140ºC. For convenience, the compression efficiencies were assumed constant for all compressor stages and equal to 80%, which can be considered as a relatively conservative estimate. The mechanical efficiency was set to 95%. Furthermore, it has been assumed that an after-cooler is installed at the discharge of the compressor station with the temperature set-point of 40ºC to protect the pipeline external coating from damage. It will also help reduce the pressure drops along the pipeline, since the CO\textsubscript{2} mixtures will be flowing at a higher density and thus with a lower velocity.
The effect of CO$_2$ mixture composition on the flow is illustrated in Figure 12. This figure shows the flow rates gradually approach their steady state values, but the flow rate is significantly affected by the gas composition, and the differences occur until the flow reaches the steady state condition. While the mass flow rates of the Oxyfuel and Pre-combustion streams slowly reach steady state condition, the mass flow rate of the Post-combustion mixture shows much faster approach to its steady state value, and, as a result of relatively low impurity concentration, nearly identical to that of CO$_2$ fluid.
Figure 13 shows the compressor station discharge pressure necessary to maintain dense phase in the pipeline under transient conditions. In case of Oxyfuel stream the discharge pressure must be considerably higher than for the remaining streams. This occurs because of higher critical pressure and larger pressure variations along the saturation curve of the Oxyfuel mixture, compared to other CO$_2$ mixtures (Fig. 11). Therefore, the selection of Oxyfuel capture technology is expected to generate higher operational costs of running of the transmission infrastructure. The fluctuation amplitude of Pre-combustion and Post-combustion CO$_2$ mixtures remains approximately constant, comparable to that of CO$_2$ fluid. The impurity combination in the Oxyfuel mixture, however, causes the difference in pressure drop to become slightly higher, in particular when the throughput increases.

As Figure 14 depicts, the computed temperatures at the delivery node behave differently over a twenty-four hour period of time. While in the case of pressure, the mixtures show different but similar behaviour during several mass flow rate changes, this cannot be said about the temperature variations at the end of the pipeline. At the initial conditions, the outlet temperatures of the CO$_2$ and the Post-combustion mixture were 7.5°C and 7.7°C, respectively. This compares to the temperatures of 9.3°C and 11.8°C obtained for the Oxyfuel and Pre-combustion mixtures, respectively. Furthermore, different amplitudes and phases of the temperature variations were seen in the solutions, i.e. the temperature changes propagate along the pipe at different speeds. Above differences seem to be caused by the underlying effects of different heat capacity rates of the CO$_2$ mixtures. In order to perform a systematic evaluation of the effect of heat capacity, the temperature and heat capacity profiles along the pipeline at the initial conditions were calculated and illustrated in Figs. 15 and 16. Furthermore, Table 3 containes the values of the specific heat at constant pressure as a function of distance obtained from REFPROP database at the initial conditions. It is worth noting that in the case of CO$_2$ and post combustion mixture the heat capacities are monotonically decreasing along the pipeline, while in the case of precombustion and oxyfuel mixtures it shows a non-monotonic behavior. The comparison of both profiles shows that the temperature gradient along the pipeline is mainly driven by the magnitude of heat capacity rates, i.e. the higher the heat capacity of the fluid stream, the lower the temperature gradient along the pipeline. Moreover, in terms of temperature changes, the thermal model of the pipeline includes the heat capacity that varies with time, as for example in Fig. 17, where time evolution of heat capacity (effect of pressure) at the inlet node of the pipeline can be seen. The amplitude of heat capacity variations of the Oxyfuel and Pre-combustion streams is noticeably lower than the amplitudes of the remaining streams, which might be the cause of a lower temperature changes of these CO$_2$ mixtures.
Fig. 14. Variation of temperature at the delivery node.

Fig. 15. Temperature distribution along the pipeline (initial condition).

Fig. 16. Changes of heat capacity along the pipeline at $t = 0$.

Fig. 17. Variation of heat capacity at the pipeline inlet.
Table 3. Specific heat at constant pressure as a function of distance

<table>
<thead>
<tr>
<th>Distance (km)</th>
<th>Specific heat at constant pressure $c_p$ (kJ/kg K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$CO_2$</td>
</tr>
<tr>
<td>1</td>
<td>8.2086</td>
</tr>
<tr>
<td>10</td>
<td>6.3750</td>
</tr>
<tr>
<td>20</td>
<td>4.6157</td>
</tr>
<tr>
<td>30</td>
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<tr>
<td>40</td>
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</tr>
<tr>
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</tr>
<tr>
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<td>2.4804</td>
</tr>
<tr>
<td>110</td>
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<td>120</td>
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<tr>
<td>130</td>
<td>2.3832</td>
</tr>
<tr>
<td>140</td>
<td>8.2086</td>
</tr>
</tbody>
</table>

The different phases of the temperature variations in the mixtures (Fig. 14) result from the combined effects of pressure on properties and transport delays within the pipeline. As an example, the inverse pressure dependence of the specific heat at constant pressure of Pre-combustion and Post-combustion streams can be observed in Fig. 17.

The comparison of compression power for different $CO_2$ mixture compositions under transient conditions is illustrated in Fig. 18. The compressor suction pressure of 0.2 MPa, and suction temperature of 40ºC were assumed. The total energy demand (compressor work input) for the 24h simulation period in case of Oxyfuel stream was 588 MWh, compared to 524 MWh in case of the $CO_2$ stream. For Pre-combustion and Post-combustion streams, the figures were 541 and 524 MWh, respectively. Therefore, the total energy demand for the transportation of Oxyfuel and Pre-combustion mixtures in the simulation period was, respectively, 12.2% and 3.2% higher than that of Post-combustion mixture, which, in turn, appeared to be equal to the total energy demand of a $CO_2$ fluid. One may reasonably suppose that fuel and electric power expenditures will generate higher operational costs, both to run the compressors and for the after-cooler facilities in case of Oxyfuel and Pre-combustion technologies.
5. Conclusions
The results of the transient simulation of the CO$_2$ pipelines performed in this study indicate that the CO$_2$ mixtures from different capture technologies show different dynamic behaviour during pipeline transport. In particular, the CO$_2$ mixture from separation plants using Oxyfuel technology presents considerable different pressure-temperature conditions, as well as compressor station capacity and fuel consumption, in comparison to Post-combustion and Pre-combustion processes.

Given the intermittency of the renewable sources, it seems reasonable to assume a variable delivery rates of CO$_2$ in separation plants, since fossil fuel based power plants will have to provide the necessary swing capacity. Therefore, the detailed design of pipeline infrastructure for CO$_2$ sequestration should be on the premise that the flow is unsteady. The length and the size of the potential transmission networks causes that the prediction of operational data should be done using modelling and simulation techniques to ensure cost effective design, as well as safe and efficient operation of CO$_2$ pipelines.

References


