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Steady-state simulation of pipeline networks for carbon dioxide transportation

Symulacja stanu stacjonarnego sieci rurociągów do transportu dwutlenku węgla

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Keywords: *pipeline networks; hydraulic modeling; single-phase flow; CO_2 impurities; composition tracking; non-pipe elements*

Abstract

In the paper we solve a single-phase steady-state, nonisothermal flow model with composition tracking that incorporates the GERG-2008 equation of state. The solver enables evaluation of the deliverability of the pipeline system under varying CO_2 stream compositions. We considered pure CO_2 and CO_2 mixtures containing impurities obtained from pre-combustion and post-combustion carbon capture technologies. We investigated the influence of impurities, pipe inclination, and heat transfer between the CO_2-rich stream and its surroundings. The network model was solved using the Newton loop-node method coupled with the non-pipe element model in matrix notation.

Słowa kluczowe: *sieci rurociągowe; modelowanie hydrauliczne; przepływ jednofazowy; zanieczyszczone CO_2; śledzenie składu; elementy nierurowe*

Streszczenie

W artykule rozwiązujemy jednofazowy nieizotermiczny model przepływu w stanie ustalonym, ze śledzeniem składu, wykorzystując równanie stanu GERG-2008. Solver umożliwia ocenę wydajności systemu rurociągowego przy zmiennym składzie strumienia CO_2. Rozważaliśmy czysty CO_2 oraz mieszaniny CO_2 zawierające zanieczyszczenia otrzymywane z technologii wychwytywania dwutlenku węgla przed spalaniem i po spalaniu. Zbadaliśmy wpływ zanieczyszczeń, nachylenia rurociągu oraz wymiany ciepła między strumieniem bogatym w CO_2 a otoczeniem. Sieć rurociągowa została rozwiązana przy użyciu metody pętli Newtona w notacji macierzowej sprzężonej z modelem elementów niererurowych.

Introduction

Carbon dioxide has been identified as the main anthropogenic greenhouse gas (GHG), accounting for nearly three-quarters of total GHG emissions globally. A significant share of those CO_2 emissions is the result of fossil fuel usage and industrial operations [3,20]. Carbon capture, utilization and storage (CCUS) is a promising way of abating those emissions and has been recognized as necessary to achieving EU's goals of reaching net-zero emissions by 2050 [2,24]. Furthermore, combining bioenergy with carbon capture and storage technology allows for clean energy production with net carbon removals from the atmosphere [6].

Transportation of the CO_2 from emitters to carbon sinks is a vital part of the carbon capture chain. For the purpose of large scale capture applications, pipeline networks are the preferred mode of transportation. CO_2 is typically proposed to be transported as supercritical/dense phase fluid [15,21], since this provides benefits of lower viscosity, similar to gaseous state, and higher density comparable to liquid. Current industrial CO_2 transportation requires maintaining high operating pressure conditions, above the critical point.

Existing applications of CO_2 pipeline modeling include route planning, pipeline network design, transport infrastructure sizing, and flow assurance studies. Modeling is critical for planning regional or national CO_2 pipeline networks, such as those in the US (e.g., the Intermountain West region and nationwide [25]) or Europe (e.g. Germany [25]). It helps determine optimal routes and connections between CO_2 sources and sinks. The design and optimization of pipeline networks through the use of rigorous hydraulic equations enables detailed infrastructure sizing, thanks to the accurate description of the CO_2 flow within the pipelines in an optimisation model [8,14]. Managing operations and surge events in supercritical or dense phase CO_2 pipelines requires precise modeling to predict pressure and temperature variations, prevent hydrate formation or phase changes, and ensure system deliverability [10].

A significant number of review articles have been published in recent years on the CCUS value chain.

A number of studies concerned the hydraulic modeling of CO_2 pipelines under steady-state conditions for design purposes. McCoy and Rubin [13] developed a supercritical CO_2 pipeline model meant for determining diameter, calculating the cost and economics of the pipeline, linking the design of pipelines with the cost of construction and operation to arrive at the total cost of CO_2 transport. Similarly in [4] authors used steady state flow modeling with the aim of reducing the network cost per tonne of CO_2 avoided. Another steady-state modeling was applied by Skaugen et al. in [22] on a 500 km long

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pipeline system which includes compressors, with the objective of analyzing the impact of impurities in the CO_2 mixture on operating costs, capital costs and energy consumption of CCS pipeline. The authors showed that the presence of impurities could increase the operating costs by as much as 40%. Teh et al. [23] investigate the difference between dense-phase and supercritical CO_2 pipeline flow and highlight the importance of ambient temperature and heat transfer and pipeline elevation in flow modeling. They considered a 90 km pipeline with 3 compressors/pumps simulated in steady state in Aspen Hysys with Peng-Robinson equation of state. They found that dense phase fluid can accommodate the impact of elevation change better than supercritical fluid and claim that dense phase could reduce the operating costs of the pipeline. Martynov et al. [12] compared the integral models of pressure and temperature drop in a pipeline, mostly adapted from the hydrocarbon industry, with results obtained from numerical solution of mass, momentum and energy equations. They concluded that in the case of supercritical CO_2 flow the impact of temperature change along the pipeline on pressure drop could account for deviation of up to 30% compared to isothermal model. Additionally, calculations based on the integral models are conservative, but accurate and can be used in pipeline network design. In [7] a net energy analysis was performed for a proposed country-wide CCS network. The authors have identified a scarcity of research regarding simulation of supercritical CO_2 flows in complex network structures.

An important aspect of the shared CO_2 transport infrastructure, particularly in developments of CCUS for industrial clusters, is that the transportation involves more destinations, tying several emitters together to a shared transport infrastructure. Composition tracking tools and a common CO_2 quality specifications considering the risk of chemical reactions between the different CO_2 streams are necessary to reduce the risk of corrosion and flow assurance issues. Given the complexity of fluid characterization and flow property assessments, in this paper we focus our effort on the correct estimation of the effect of impurities on steady state hydraulic and thermal performance analyses. We illustrate that this estimation can only be done with the adequate CO_2 transport network model. A mathematical engine for simulating hydraulic behavior of gas transport networks under isothermal flow conditions, incorporating controllable elements, such as sources, compressors, regulators, and valves has been formulated in [17]. In the subsequent work [18] this engine has been equipped with GIS based GUI system allowing for simple data input, easy-to-analyze results output and developed into software package SimNet for steady-state simulation of gas networks of arbitrary structure [5]. In this work, we focus on extending the mathematical engine mentioned above by a combined model composed of GERG-2008 equation-of-state compositional model for the CO_2-rich mixtures [9], and a composition tracking model incorporating nodal mixing rules. The model considers the constraints and control of the most important facilities in the CO_2 transport system, such as compressor/pump stations and storage site facilities. The use of a nonisothermal flow model suitable for non-planar network structures is inevitable in CO_2 pipeline networks, due to high density of the transported fluid and the thermodynamic nature of the prevailing processes in CO_2 transport systems, i.e. significant effect of temperature on density.

Steady-state CO_2 network simulation problem

The SimNet package, described in detail in [16,17,18], was used to simulate steady states in the carbon dioxide pipeline network.

In the analyzed case, the following equation was used to simulate the steady state:

$$p_i^2 - p_j^2 = \Phi_i[(Q_n)_k] = K_k(Q_n^2)_k \tag{1}$$

where

$$K_k = ZR\bar{T}\lambda L\rho_n^2 A^{-2} D^{-1} \tag{2}$$

whereby

Z is the compressibility factor, R is the specific gas constant, $\bar{T}$ is the mean gas temperature, λ is the Darcy friction factor, L is the pipe length, P_n is the density of the gas at standard conditions, A is the cross-sectional inside area of the pipe and D is the internal diameter of the pipe.

Equation (6) holds for a planar network. For non-planar pipelines the flow equation takes the form

$$p_i^2 - e^s p_j^2 = ZR\bar{T}\lambda L_e\rho_n^2 A^{-2} D^{-1}(Q_n^2)_k \tag{3}$$

where $s = 2g(H_j - H_i)/(ZRT_j)$, while H_j is the elevation of the receiving node, H_i is the elevation of the sending node and L_e is the equivalent length of the pipe, calculated from the formula $L_e = L(e^s - 1)/s$.

Maintaining high enough pressure for dense phase / supercritical state CO_2 requires gas compression causing the CO_2 temperature to rise. The temperature of the receiving node j of pipeline k can be calculated the following equation:

$$T_j = \frac{\beta}{\beta+\gamma}\left[T_{amb} - T_{amb}e^{-(\beta+\gamma)L}\right] + T_i e^{-(\beta+\gamma)L} \tag{4}$$

where

$$\beta = \frac{U}{\pi c_p D\rho_n Q_n},\ \gamma = \frac{\eta_{JT}\lambda ZR\rho_n^2 Q_n|Q_n|}{2\bar{p}DA^2}$$

whereby

U is the overall heat transfer coefficient, C_p is the specific heat at constant pressure, T_{amb} is the ambient temperature and η_{JT} is the Joule-Thomson coefficient

$$\eta_{JT} = \frac{1}{c_p}[T(\frac{\partial v}{\partial T})_p + v] \tag{5}$$

where v is the specific volume of the fluid. The average temperature along the length of the pipe k in equation (2) can be calculated using equation:

$$\bar{T}_k = \frac{1}{L}\int_0^L T\ d = \frac{1}{L}\left\{\frac{\beta}{\beta+\gamma}T_{amb}L + \left[\frac{T_i}{\beta+\gamma} - \frac{T_{amb}\beta}{(\beta+\gamma)^2}\right]\left[1 - e^{-(\beta+\gamma)L}\right]\right\} \tag{6}$$

On the other hand, for high-pressure gas networks the average pressure is calculated from the following expression

$$\bar{p} = 2/3\left[p_i + \frac{p_j^2}{p_i + p_j}\right] \tag{7}$$

Relations for average temperature and pressure were used for calculation of thermodynamic properties, such as compressibility factor, specific heat at constant pressure and Joule-Thomson coefficient.

Composition tracking

For a perfect mixing of the components of the incoming gas, the mass balance equation at node p takes the form

$$\sum_p (\rho_n^I)_i (Q_n^I)_i (x_j^I)_i = \sum_p (\rho_n^O)_i (Q_n^O)_i (x_j^O)_i \tag{8}$$

where x_j is the mass fraction of the j-th component of the mixture, while I indicates the streams entering the node and O the ones leaving it.

A similar approach is taken for the energy balance in nodes. The energy balance equation is expressed as follows

$$\sum_{p}(\rho_n^I)_i(Q_n^I)_i h_i^I = (\rho_n)_p h_p \sum_{p}(Q_n^O)_i \tag{9}$$

where h denotes the specific enthalpy. Calculating nodal temperature T_p and entering stream enthalpy involves performing flash calculations of temperature in terms of enthalpy and pressure $T = T(h,p)$, and enthalpy as a function of pressure and temperature $h = h(T,p)$ using a selected equation of state.

This mixing rule is valid for each property that can be represented by linear relations in the components. Finally, for all nodes in the network, the following set of algebraic linear equation can be written:

$$\mathbf{Gx} = \mathbf{b} \tag{10}$$

where **G** is an N by N matrix containing mass flows, **x** is the vector with the nodal property, and **b** is the right-hand side vector containing the sums of products of the property and the mass flow of supplies.

Compressor model

Compression running costs are the main expenses associated with the operation of a pipeline network. In addition, aftercoolers are installed at compressor outlets to lower the fluid temperature, thus reducing pipeline wear and increasing the capacity of the pipeline. Assuming the kinetic and potential energy changes are negligible, the compressor power input is calculated as follows

$$P = \rho_n Q_n \frac{1}{\eta_{is}}\left(h(p_{out}, s_{in}) - h(p_{in}, T_{in})\right). \tag{11}$$

where η_{is} is the isentropic efficiency of the compressor, h is the specific enthalpy and s is the specific entropy, while the subscripts "in" and "out" denote the suction and discharge ends of the compressor, respectively. The parameters p_{in}, T_{in}, p_{out} are obtained from the simulation results, while the inlet entropy is calculated as $s_{in} = s(p_{in}, T_{in})$. The aftercooler cooling demand is calculated from the following expression

$$Q = \rho_n Q_n\left(h(p_{ac}, T_{ac}) - h(p_{out}, T_{out})\right) \tag{12}$$

where the subscript "ac" denotes the outlet of the cooler.

In the next section, firstly, the simulation framework for the CO_2 networks presented in this study has been benchmarked against Pipesim flow modeling software [19], using data from a hypothetical but realistic multi-source transmission system. This is followed by an assessment of the effect of simplifying assumptions, such as isothermal flow conditions and the lack of impurities in the transported fluid, on the compression power input for various network structures. The lack of existing large-scale pipeline networks transporting impure CO_2 streams, and consequently the unavailability of measurement data, precludes validation of numerical models using real data.

Simulation results

The aim of the research was to simulate flow in a hypothetical transmission system with multiple sources. The impact of model simplifications such as isothermal flow conditions and the absence of contaminants in the transported fluid was investigated. The power consumption of compressors for different network structures was also examined. The research was conducted using SimNet and Pipesim software.

The network structures with the location of the source and delivery nodes are shown in Figure 1 and in the graphical user interface of the corresponding software packages in Figures 2 and 3. The capacity of each network was studied both in the supercritical/dense phase and in the gaseous phase conditions.

Both networks consist of 49 source emitters divided into two groups: the pre-combustion emitters, which include hydrogen production sites and fertilizer plants, and the post-combustion consisting of coal and natural gas-fired power plants as well as cement production sites. Four impurities were present in the CO_2-rich streams with concentration for each source presented in Table 1 with limits based on [3].

Comparison of pressure and mole fraction results are presented in Table 2. The pressure results in Simnet deviates from Pipesime results in the dense phase scenario, whilst the gasous phase results show smaller deviations of around 1%. The composition results align very well for all scenarios with hydrogen presenting highest deviation of 1.19%. Simulation with Simnet also results in lower required power input by 13-20% for analyzed scenarios.

Table 1 Composition of captured mixtures (mole fractions).

Tabela 1 Skład wychwytywanych mieszanin (ułamki molowe).

Mixture	CO_2	N_2	Ar	H_2	CH_4
Post	97.2%	2.4%	0.4%	0.0%	0.0%
Pre	96.1%	2.0%	0.4%	0.5%	1.0%

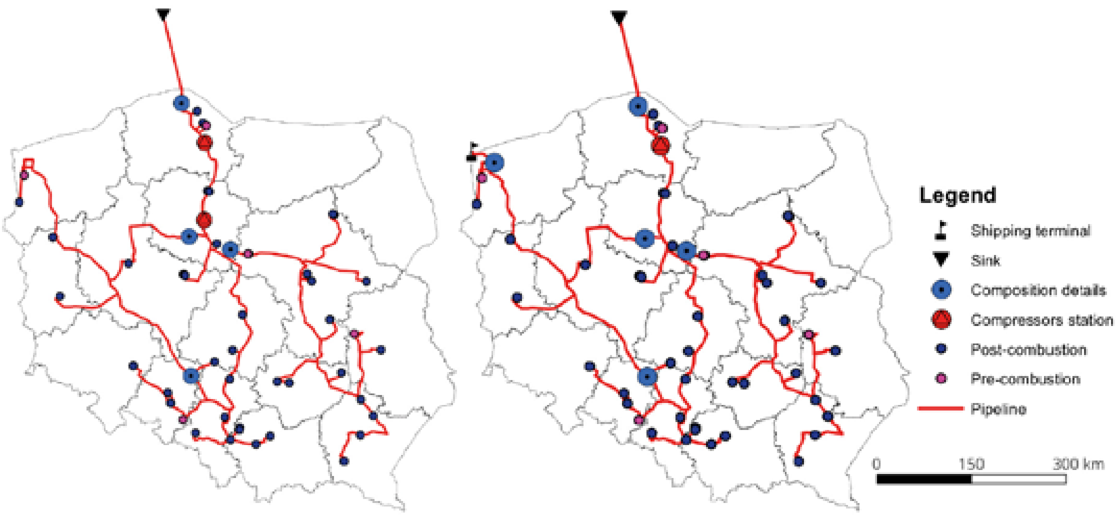

Fig. 1 Network structure in Example 1 (left) and Example 2 (right)

Rys. 1 Struktura sieci w Przykładzie 1 (lewy) i Przykładzie 2 (prawy)

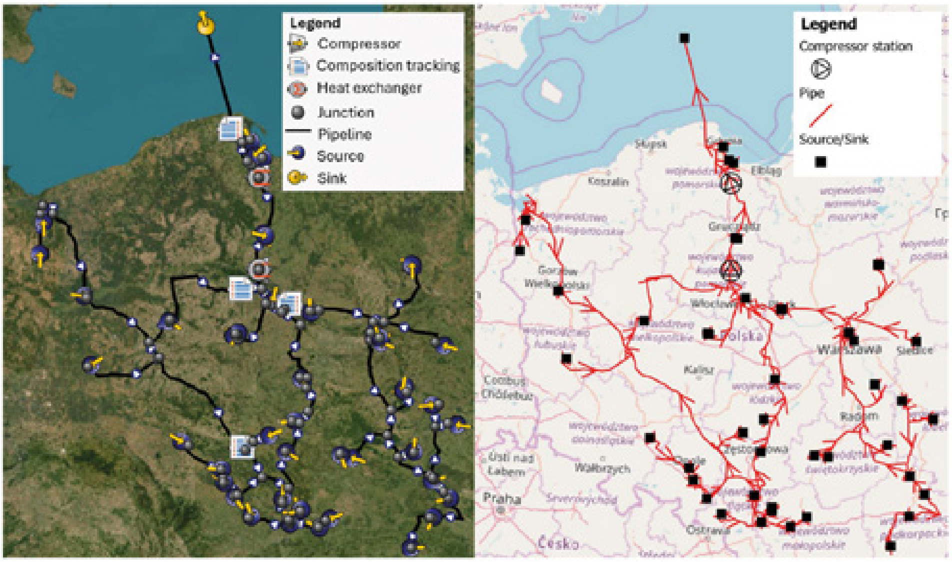

Fig. 2 Visual representation of the network structure in Example 1, Pipesim (left) and SimNet (right)

Rys. 2 Reprezentacja wizualna struktury sieci dla Przykładu 1, Pipesim (lewy) i SimNet (prawy)

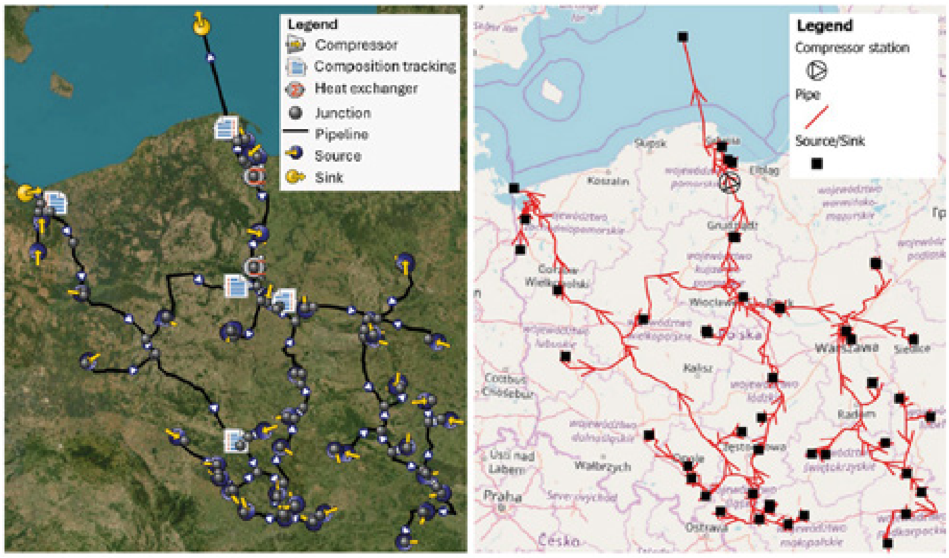

Fig. 3 Visual representation of the network structure in Example 2, Pipesim (left) and SimNet (right)

Rys. 3 Reprezentacja wizualna struktury sieci dla Przykładu 2, Pipesim (lewy) i SimNet (prawy)

Table 2 Percentage difference between Pipesim and Simnet results

Tabela 2 Różnice procentowe pomiędzy wynikami z Pipesima i z SimNeta

Property	Example 1		Example 2	
	Dense phase	Gaseous phase	Dense phase	Gaseous phase
Pressure	4.85%	0.85%	4.88%	1.25%
CO_2 fraction	0.00097%	0.00057%	0.00075%	0.00027%
N_2 fraction	0.015%	0.0086%	0.011%	0.004%
H_2 fraction	0.91%	0.54%	1.19%	0.37%
CH_4 fraction	0.91%	0.54%	1.11%	0.39%
Compressor power	-19.1%	-17.2%	-13.5%	-18.4%

Effect of nonisothermal flow conditions on compressor power input

Most flow models presented in the literature assume isothermal flow conditions, therefore a comparison of the results of compressor power inputs for isothermal and non-isothermal flow models was carried out. Under isothermal flow conditions, the temperature of the transported CO_2-rich fluids was set to 8°C, which is the temperature of the surroundings of the pipeline. The results are shown in Table 3 In the case of gaseous phase flow, the differences in compressor power input are negligible for the first example and small (at the level of a few percent) for the second example. This is mainly due to the low mass flow rates of the gas in the pipelines and the rapid decrease of the gas temperature along the length of the pipeline to near ambient temperature. In the case of dense-phase flow, the differences are significant and reach tens of percent. The isothermal flow model underestimates the compressor power input, which is a consequence of lower pressure drops in the network due to the higher density and lower flow velocity of the colder fluid.

Table 3 Compressor power input under isothermal flow conditions and comparison with respect to the results of the non-isothermal flow model.

Tabela 3 Moc sprężarek przy przepływie izotermicznym oraz porównanie z wynikami dla przepływu nieizotermicznego.

Isothermal flow	Compressor	Example 1		Example 2	
		Dense phase	Gaseous phase	Dense phase	Gaseous phase
Compressor power	Downstream	32.4 MW	18.6 MW	9.66 MW	10.0 MW
	Upstream	36.0 MW	18.5 MW	-	-
Percentage difference	Downstream	-19.8	-0.45	-24.5	3.42
	Upstream	-11.5	0.37	-	-

Table 4 Compressor power input and aftercooler load for pure CO2 stream and comparison with respect to the impure stream; values in parentheses indicate cooling demand.

Tabela 4 Moc sprężarek oraz chłodnicy dla przepływu czystego CO_2 oraz porówanie wyników w stosunku do zanieczyszczonego CO_2

Pure CO_2	Compressor	Example 1		Example 2	
		Dense phase	Gaseous phase	Dense phase	Gaseous phase
Compressor power	Downstream	35.2 (12.13) MW	17.9 (13.8) MW	10.4 (0) MW	9.27 (0.16) MW
	Upstream	38.26 (0) MW	17.7 (11.8) MW	-	-
Percentage difference	Downstream	-12.9 (-67.0)	-4.11 (-1.12)	-18.7 (-)	-4.5 (-60.1)
	Upstream	-5.88 (-)	-4.03 (-1.90)	-	-

Effect of impurities in the CO_2 stream on compressor power input and aftercooler load

The impact of the presence of impurities in the CO_2 stream on compressor power input was also studied. Both networks were simulated under the assumption that pure CO_2 is transported in an amount equal to the amount of CO_2 transported in the impure stream. The results of the compressor power input and the cooling load for the pure stream along with the differences with respect to the impure stream are presented in Table 4. The results show that the compression power decreases with increasing CO_2 stream purity, confirming the results reported in [11]. As can be seen, the impact is more pronounced in the case of a dense-phase flow with a reduction of about 13% in the power required by the downstream compressor. The notable large reduction in the cooling power requirement is due to the fact that the cooler inlet temperatures for pure CO_2 stream and the impure stream are 31.2°C and 32.7°C, respectively, while the cooler outlet temperature setpoint is 30°C.

Functionality and computational complexity

SimNet software allows for setting the compressor inlet pressure as an initial condition for the compressor station. This ensures that the pressure does not fall below a pressure setpoint value at any node in the network, preventing two-phase flow conditions in networks designed for supercritical/dense-phase flow. This functionality is not available to users of Pipesim software, where only pressure difference, pressure ratio, outlet pressure, or power input can be specified for a non-pipe element, with no control over the risk of phase transition within the fluid flow in the network

The investigation also concerned the scalability of the network model in relation to the complexity of the network structure. The network from Example 2 was extended with additional pipelines that formed 8 independent loops. The new pipelines were assumed to also be routed in existing natural gas pipeline corridors. Two new CO_2 delivery nodes are also present in the network. The structure of the network is shown in Figure 5. The network simulation times are shown in Table 5 and are the result of averaging of 5 runs of simulation calculations. The complexity of the network is a significant factor that affects the computation time of Pipesim software, doubling the required computation time. In the case of Simnet software, no additional computational burden is seen to solve the network. There are two reasons for this occurrence, firstly, the compressor inlet pressure setpoint allows a constraint to be imposed on the lowest pressure value in the network above the critical pressure, eliminating the need for flash calculations to determine the presence of phase transition. The second factor is the use of symbolic factorization of sparse matrices so that only non-zero elements need to be stored and operated on in memory. Sparse matrix methods for network simulation problems based

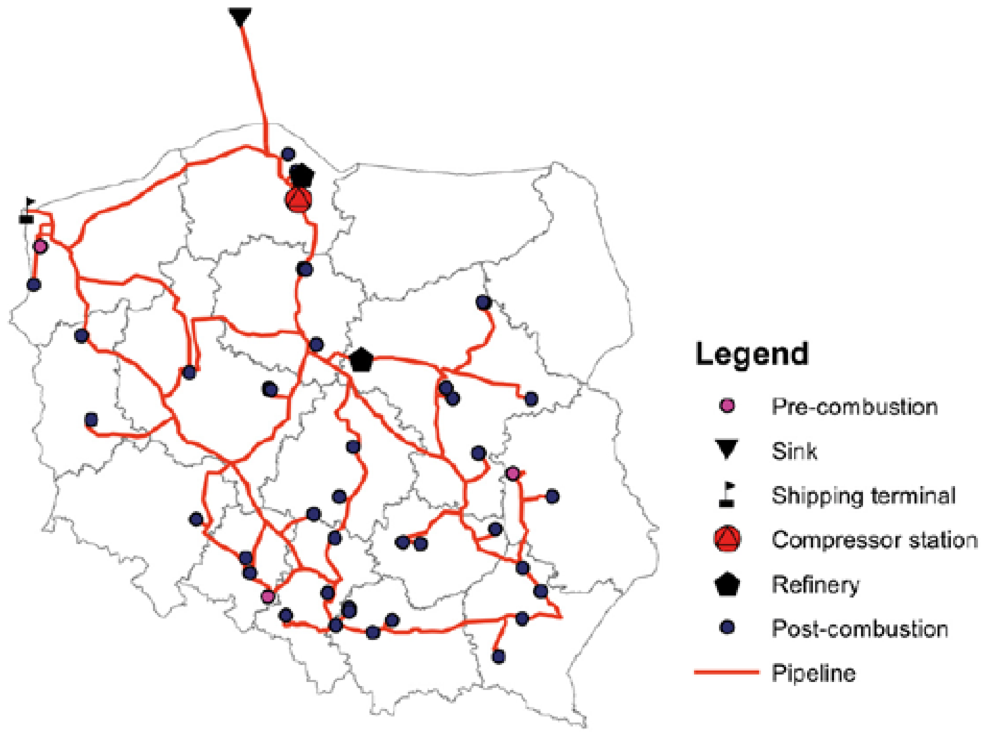

Fig. 4 Structure of the network for computational complexity study

Rys. 4 Struktura sieci wykorzystana przy analizie efektywności obliczeniowej on node re-ordering are detailed in [16]. Furthermore, tests have shown that the execution times scale linearly with the number of discretization sections in the network.

Table 5 Simulation execution time for dense-phase flow.

Table 6 Czas obliczeniowy symulacji dla przepływu w fazie gęstej

Time, s	Example 1	Example 2	Multiple loops
Pipesim	157	138	293
SimNet	1.68	1.76	1.86

Conclusion

In this work, we have integrated the GERG-2008 equations of state and composition tracking into a steady-state, nonisothermal, single-phase flow model that uses efficient Newton loop-node coupling. The solver is capable of simulating networks of any size and topology, including complex loop structures and non-pipe elements such as compressors, valves, and pressure/flow regulators. The GERG 2008 equation-of-state compositional model and composition tracking functionality ensure an accurate description of fluid behavior in terms of fluid property modeling. The model accounts for heat transfer, Joule-Thompson cooling, and node elevation differences. By modeling the entire system as a network, the interdependency of complex network structures and non-pipe elements can be accounted for, and the deliverability of the system can be determined.

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