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A COMPARISON BETWEEN PSRK AND GERG-2004 EQUATION OF STATE FOR SIMULATION OF NON-ISOTHERMAL COMPRESSIBLE NATURAL GASES MIXED WITH HYDROGEN IN PIPELINES

PORÓWNANIE RÓWNAŃ STANU OPRACOWANYCH WEDŁUG METODY PSRK ORAZ GERG-2004 WYKORZYSTANYCH DO SYMULACJI ZACHOWANIA ŚCIŚLIWYCH MIESZANIN GAZU ZIEMNEGO I WODORU W RUROCIĄGACH, W WARUNKACH PRZEPŁYWÓW NIE-IZOTERMICZNYCH

In this work, the GERG-2004 equation of state based on a multi-fluid approximation explicit in the reduced Helmholtz energy is compared with the predictive Soave-Redlich-Kwong group contribution method. In the analysis, both equations of state are compared by simulating a non-isothermal transient flow of natural gas and mixed hydrogen-natural gas in pipelines. Besides the flow conditions also linepack-energy and energy consumption of the compressor station are computed. The gas flow is described by a set of partial differential equations resulting from the conservation of mass, momentum and energy. A pipeline section of the Yamal-Europe gas pipeline on Polish territory has been selected for the case study.

Keywords: GERG-2004, PSRK method, hydrogen, pipeline, unsteady gas flow

W artykule dokonano porównania wyników uzyskanych przy wykorzystaniu równania stanu GERG-2004 opartego na jawnym przybliżeniu wyników dla wielu cieczy w oparciu o zredukowaną energię Helmhotza oraz wyników uzyskanych w oparciu o metodę Soave-Redlich Kwonga. Obydwa równania stanu porównano poprzez przeprowadzenie symulacji stanów przejściowych przepływów gazu ziemnego oraz mieszanin gazu ziemnego i wodoru w rurociągach w warunkach przepływów nie-izotermicznych. Oprócz warunków przepływu, określono energię w napełnionym układzie oraz zużycie energii przez stację kompresora. Przepływ gazu opisano zbiorem równań różniczkowych cząstkowych, wyprowadzonych w oparciu o prawa zachowania masy, pędu i energii. Jako studium przypadku wybrano fragment rurociągu jamalskiego (Yamal- Europa) przebiegającego przez terytorium Polski.

Słowa kluczowe: GERG-2004, metoda PSRK, wodór, rurociąg, nieustalony przepływ gazu

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1. Introduction

The accurate knowledge of thermodynamic properties of natural gas is important in a wide range of engineering applications. The choice of equation of state may have a great impact on calculations in custody transfer and transmission and distribution applications. The latter comprises equations governing the flow conditions in the pipeline, estimation of linepack, compressor and heat exchanger design, orifice plate and sonic nozzle metering and conversion of gas volumes to the reference state. One group of models uses excess properties to describe the behavior of mixtures. Gmehling (1993) used the excess Gibbs free energy and Huron and Vidal (1979) and Heidemann (1996) used the excess Helmholtz free energy. The other more recent equations of state are introduced by Tillner-Roth (1993) and Lemmon (1996). These are based on multi-fluid approximations at which the equations are made explicit in the Helmholtz free energy. A well-known a multi-fluid approximation is GERG-2004 (Kunz, et. al., 2007).

In this work, the PSRK (Predictive Soave-Redlich-Kwong) group-contribution method (Holderbaum & Gmehling, 1991; Fischer & Gmehling, 1996; Gmehling et al., 1997; Horstmann et al., 2000) is compared with GERG-2004 (Kunz et al., 2007) for the simulation of transient flow conditions in natural gas pipelines. In the case study not only natural gas is considered but also natural gas mixed with hydrogen. The latter mixture is motivated due to the fact that hydrogen is considered as a promising alternative in our future energy demand. A first step towards a hydrogen economy would be to utilize existing distribution gas pipelines by mixing the natural gas with less than 17 vol% of hydrogen (Haeseldonckx & D'haeseleer, 2007). Besides the flow conditions, linepack and energy consumption of the compressor station are also computed.

Nomenclature

Roman symbols

A – Cross-sectional area,
a – Equation of state mixture parameter,
a_s – Isentropic wave speed,
b – Equation of state mixture parameter,
$c_i^{[1,2,3]}$ – Mathias-Copeman coefficients,
c_p – Isobaric heat capacity,
c_p^0 – Ideal isobaric heat capacity,
d – Diameter pipeline,
$E_{c,tot}$ – Total energy consumption compressor,
$E_{p,tot}$ – Total linepack-energy,
f – Friction factor,
g – Gravitational acceleration,
g_0^E – Excess Gibbs energy,
$H_{s,i}$ – Higher heating value of component i,
L – Pipeline length,
$\dot{m}$ – Mass flow rates,
M – Molar mass,
M_p – Linepack,

N	–	Number of components in the mixture,
n_i	–	Concentration of component i,
p	–	Gas pressure,
p_c	–	Critical pressure,
p_i	–	Inlet pressure compressor,
p_o	–	Outlet pressure compressor,
q	–	Heat flow into the pipe,
q_1	–	Mixing rule constant,
q_n	–	Gas flow at normal conditions,
R	–	Gas constant,
R_e	–	Reynolds number,
R_s	–	Specific gas constant,
t	–	Time,
T	–	Gas temperature,
T_c	–	Critical temperature,
T_i	–	Inlet temperature compressor,
T_r	–	Reduced temperature,
T_s	–	Soil temperature,
U	–	Overall heat transfer coefficient,
v	–	Velocity,
V	–	Molar volume,
w	–	Frictional force per unit length and time,
W_t	–	Compressor power,
x	–	spatial coordinate,
$\bar{x}$	–	Molar composition,
z	–	Compressibility factor.

Greek symbols

α	–	Equation of state mixture parameter, reduced molar Helmholtz free energy,
δ	–	Reduced density,
ε	–	Compression ratio, pipeline roughness,
η_m	–	Mechanical efficiency,
η_p	–	Polytropic efficiency,
θ	–	Inclination angle of the pipe,
κ	–	Isentropic exponent,
μ	–	Dynamic viscosity,
ρ	–	Density,
τ	–	Inverse reduced temperature.

2. Governing equations

2.1. Non-isothermal transient flow model

When simulating pipeline systems, it is convenient to assume that the flow is steady because it is easier to solve and under certain conditions the results are adequate (Chaczykowski & Osiadacz, 2012). Hence, the design and analysis should always be based on the premise that the flow is unsteady. Thorley (1987) derived from the laws of conservation of mass, momentum and energy, the basic equations describing a one-dimensional transient flow. The governing equations in term of partial differential equations are expressed as follows

$$\frac{\partial p}{\partial t} + v\frac{\partial p}{\partial x} + \rho a_s^2 \frac{\partial v}{\partial x} = \frac{a_s^2}{c_p T}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\left(\frac{q + wv}{A}\right) \tag{1}$$

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = -\frac{w}{A\rho} - g\sin(\theta) \tag{2}$$

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x} + \frac{a_s^2}{c_p}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\frac{\partial v}{\partial x} = \frac{a_s^2}{c_p p}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\left(\frac{q + wv}{A}\right) \tag{3}$$

where the isentropic wave speed is defined as

$$a_s^2 = \sqrt{\frac{zR_s T}{\left[\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right) - \frac{p}{\rho c_p T}\left(1 - \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)^2\right]}} \tag{4}$$

and the frictional force per unit length is given by

$$w = \frac{f\,v\rho|v|}{8}\pi d \tag{5}$$

The friction factor, f, is calculated from the Colebrook-White equation (Colebrook, 1939)

$$\frac{1}{f} = -2.0\log\left(\frac{\varepsilon}{3.7d} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right) \tag{6}$$

As a matter of convenience, Eqs. (1-3) can be written in terms of mass flow. This is accomplished by using the state equation for a real gas, $p/\rho = zRT$. The resulting set of equations is

$$\frac{\partial p}{\partial t} = \frac{a_s^2}{c_p T}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\left(\frac{q}{A} + \frac{\dot{m}zRT}{pA^2}w\right) - \left[\frac{\dot{m}zRT}{pA} - \frac{a_s^2\dot{m}}{pA}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\right]\frac{\partial p}{\partial x}$$
$$- \frac{a_s^2\dot{m}}{TA}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\frac{\partial T}{\partial x} - \frac{a_s^2}{A}\frac{\partial\dot{m}}{\partial x} \tag{7}$$

$$\frac{\partial T}{\partial t} = \frac{a_s^2}{c_p p}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\left(\frac{q}{A} + w\frac{\dot{m}zRT}{pA^2}\right) - \frac{\dot{m}zRT}{pA}\frac{\partial T}{\partial x} - \frac{a_s^2}{c_p}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)$$
$$\times\left[\frac{\dot{m}zR}{pA}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\frac{\partial T}{\partial x} - \frac{\dot{m}TRz}{p^2A}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\frac{\partial p}{\partial x} + \frac{zTR}{pA}\frac{\partial \dot{m}}{\partial x}\right]$$
(8)

$$\frac{\partial \dot{m}}{\partial t} = -\frac{\dot{m}}{T}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\frac{\partial T}{\partial t} + \frac{\dot{m}}{p}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\frac{\partial p}{\partial t} - \frac{\dot{m}^2 zR}{pA}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\frac{\partial T}{\partial x}$$
$$+ \left(\frac{\dot{m}^2 TRz}{p^2A}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right) - A\right)\frac{\partial p}{\partial x} - \frac{\dot{m}zTR}{pA}\frac{\partial \dot{m}}{\partial x} - w - \frac{pAg\sin(\theta)}{zTR}$$
(9)

The heat transfer, q represents the amount of heat exchanged between the gas and its surroundings per unit length and per time and is defined as follows

$$q = -\pi dU\left(T - T_s\right)$$
(10)

2.2. Real gas effects

The transport properties are calculated from two different equations of state. First, the PSRK method, which combines the Soave-Redlich-Kwong (SRK) equation of state (Soave, 1972), incorporated with the modified Huron-Vidal first-order mixing rule (Dahl & Michelsen, 1990) is applied. The modified UNIFAC group contribution model (Hansen et al., 1991) is used as the excess Gibbs energy for the mixing rule. The SRK equation of state is given by

$$p = \frac{RT}{V - b} - \frac{a}{V(V + b)}$$
(11)

where the mixture parameter, b, is derived from the conventional linear mixing rule,

$$b = \sum_{i=1}^{n} x_i b_{ii}$$
(12)

The parameters, a and b, of component i are given by

$$a_{ii} = 0.42747\frac{R^2 T_{c,i}^2}{p_{c,i}}f\left(T_{r,i}\right)^2 \quad , \quad b_{ii} = 0.008664\frac{RT_{c,i}}{p_{c,i}}$$
(13)

where $f(T_{r,i})$ is the Mathias-Copeman correlation (Mathias & Copeman, 1983)

$$f\left(T_{r,i}\right) = \begin{cases} 1 + c_i^{[1]}\left(1 - \sqrt{T_{r,i}}\right) + c_i^{[2]}\left(1 - \sqrt{T_{r,i}}\right)^2 + c_i^{[3]}\left(1 - \sqrt{T_{r,i}}\right)^3 & \text{if } T_{r,i} < 1 \\ 1 + c_i^{[1]}\left(1 - \sqrt{T_{r,i}}\right) & \text{if } T_{r,i} > 1 \end{cases}$$
(14)

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The equation of state mixture parameter, a, is calculated from the modified Huron-Vidal first-order mixing rule,

$$\alpha = \sum_{i=1}^{n} x_i \left(\frac{a_{ii}}{b_{ii} RT} \right) + \frac{1}{q_1} \left(\frac{g_0^E}{RT} + \sum_{i=1}^{n} x_i \ln \frac{b}{b_{ii}} \right) \tag{15}$$

where $\alpha = a/bRT$ and $q_1 = -0.64663$. The Gibbs free energy, g_0^E, is calculated from the UNIFAC model.

The second equation of state used in this work is GERG-2004, which is based on a multi-fluid approximation explicit in the reduced Helmholtz energy. The basic structure of the multi-fluid approximation is

$$\alpha(\delta, \tau, \overline{x}) = \alpha^0(\rho, T, \overline{x}) + \sum_{i=1}^{N} x_i \alpha_{0i}^r(\delta, \tau) + \Delta \alpha^r(\delta, \tau, \overline{x}) \tag{16}$$

where the reduced density and inverse reduced temperature are $\delta = \rho/\rho_n(\overline{x})$ and $\tau = T_n(\overline{x})/T$. The first part in Eq. (16) is the ideal gas part followed by the contribution of the pure gases and the last part is a departure function. The latter is as a double summation over all binary specific and generalized departure functions

$$\Delta \alpha^r(\delta, \tau, \overline{x}) = \sum_{j=i+1}^{N} \sum_{i=1}^{N-1} \Delta \alpha_{ij}^r(\delta, \tau, \overline{x}) \tag{17}$$

1.3. Linepack

The volume or mass of the natural gas in the pipeline is called linepack and enables almost a continuous supply of natural gas in case of a varying demand. The linepack, M_p, changes over time due to the changes in density, ρ, and cross-sectional area, A, of the pipeline according to the expression:

$$M_p = \int_{0}^{t_f} \int_{0}^{L} \rho(x) A(x) \, dx \, dt \tag{18}$$

with position coordinate x, $0 \leq x \leq L$. The density depends on pressure, temperature and gas composition. The cross-sectional area changes due to deformation of the pipeline but can be assumed constant. The amount of energy in the pipeline is calculated by multiplying Eq. (18) with the lower heating value on weight basis.

1.4. Compressor equations

The total energy consumption of a centrifugal compressor for a defined control period is obtained in the following manner:

$$E_{c,tot} = \int_{t_0}^{t_f} W_t \cdot dt \qquad (19)$$

The compressor power is calculated as follows:

$$W_t = \frac{\dot{m}zRT_i}{\eta_p \eta_m M} \frac{\kappa}{\kappa-1} \left[\varepsilon^{\frac{\kappa-1}{\kappa}} - 1 \right] \qquad (20)$$

where, ε $(= p_o/p_i)$, is the compression ratio and, κ, the isentropic exponent.

3. Case study

For the case study, a 177 km pipe section of the Yamal-Europe gas pipeline on Polish territory is selected as test network (Fig. 1). The pipeline transports a mixture with an average molar composition of $CH_4 = 98.3455$, $C_2H_6 = 0.6104$, $C_3H_8 = 0.1572$, i-$C_4H_{10} = 0.0299$, n-$C_4H_{10} = 0.0253$, i-$C_5H_{12} = 0.0055$, n-$C_5H_{12} = 0.0040$, $N_2 = 0.0303$ and $CO_2 = 0.7918$. The amount of hydrogen added is 20 mol%, which results in a mole fraction of 0.167.
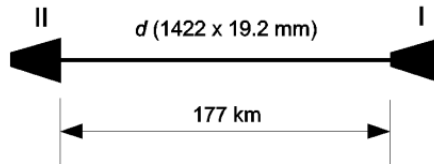

Fig. 1. Structure of the Yamal pipeline section

The pipe wall properties are shown in Table 1. The roughness of the pipe is assumed 0.016 mm. The soil temperature is 12°C and the pipeline depth is 1.5 m. The soil thermal conductivity is assumed 2.0 W/m·K. The mechanical and polytropic efficiency of the compressor are assumed constant with the values 0.97 and 0.87, respectively.

TABLE 1

Pipe wall properties

Pipe wall structure	Thickness (mm)	k (W/m·K)
Internal coating	0.5	0.52
Steel L480MB (X 70)	19.22	45.3
External coating (polyethylene)	3.0	0.4

The boundary conditions are:

$$p(0,t) = 8.4 \text{ MPa}$$
$$T(0,t) = 303.15 \text{ K}$$
$$q_n(L,t) = f(t)$$

(21)

where $f(t)$ is depicted in Fig. 2 with a time interval, $t \in [0, 24 \text{ h}]$. The variation in demand at the end of the pipeline is arbitrarily selected. The initial values for the partial differential equations are obtained by setting Eqs. (1-3) equal to zero, i.e., $\partial v/\partial t = 0$, $\partial p/\partial t = 0$ and $\partial T/\partial t = 0$. The resulting equations for a horizontal pipe are

$$\frac{\partial p}{\partial x} = \frac{a_s^2}{c_p T}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\left(\frac{q + wv}{A}\right) + \frac{a_s^2 w}{Av}\left(v - \frac{a_s^2}{v}\right)^{-1}$$

(22)

$$\frac{\partial T}{\partial x} = \frac{a_s^2}{vc_p p}\left(1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right)\left(\frac{q + wv}{A}\right) - \frac{a_s^2}{vc_p}\left(1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right)\left(-\frac{w}{vA\rho} - \frac{1}{v\rho}\frac{\partial p}{\partial x}\right)$$

(23)

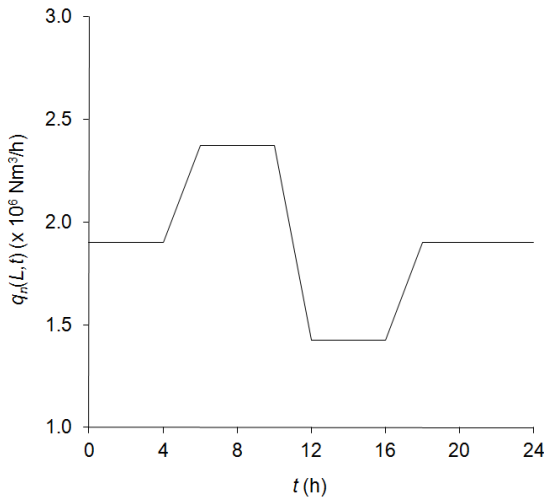The ordinary differential equations are solved by the fourth-order Runge-Kutta method.

Fig. 2. Boundary condition at $x = L$

The partial differential equations (7-9) are solved by the method of lines (Schiesser, 1991). A five-point, fourth-order finite difference approximation is used for the spatial derivatives and the stiff non-linear ODE system was solved numerically with a second-order accurate implicit Runge-Kutta algorithm. Romberg's method was used for the integration of Eqs. (18) and (19).

Fig. 3 depicts the compressibility factor computed by the PSRK method and GERG-2004 for both mixtures. It can be concluded that the deviation between de models increases at higher pressure at both 10°C and 30°C.
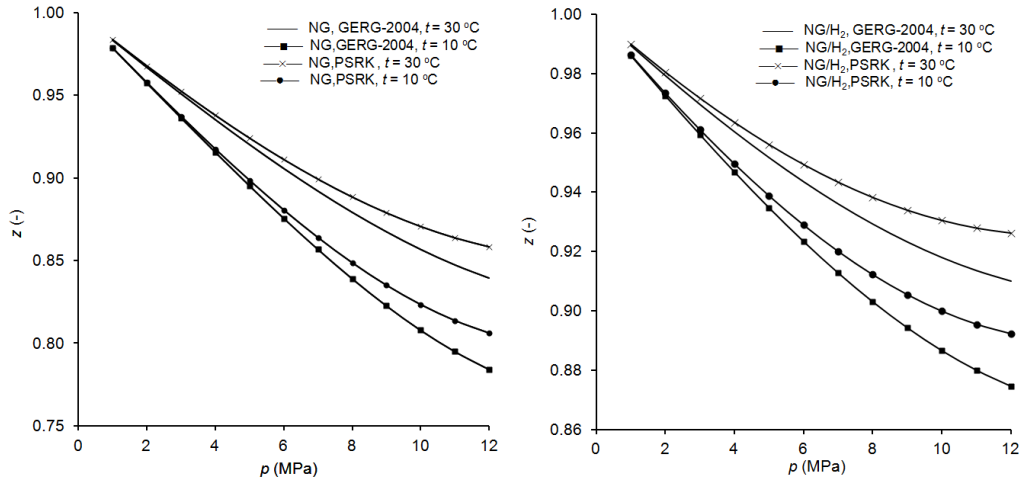

Fig. 3. Compressibility factor calculated by PSRK method and GERG-2004 for NG and NG/H$_2$

Figs. 4 and 5 show the variation of pressure and temperature at the inlet of compressor station II and in Table 2 the average values of the pressure and temperature drop are given. The use of the GERG-2004 results in a 7.1% decrease in $\Delta\bar{p}$ and an increase of $\Delta\bar{T}$ by 24% in comparison with the PSRK method. This accounts for the natural gas mixture. In case of the H$_2$/NG mixture, the corresponding values are 1.4% and 18%. The total energy consumption over the twenty-four hours period decreases by 16.2% for natural gas and 3.9% in case of the H$_2$/NG mixture. The GERG-2004 estimates a higher linepack-energy for both natural gas and natural gas mixed with hydrogen. The corresponding values are 8.5% and 1.8%, respectively.

TABLE 2

Simulation results for the 177 km pipe section

Mixture	EoS	$\Delta\bar{p}$ (MPa)	$\Delta\bar{T}$ (K)	$E_{c,tot}$ (GJ)	$E_{p,tot}$ (TJ)
Natural gas (NG)	PSRK	0.84	10.74	726.3	63.4
Natural gas (NG)	GERG-2004	0.78	13.32	608.5	68.8
H$_2$/NG (x_{H_2} = 0.167)	PRSK	0.72	11.73	602.3	56.6
H$_2$/NG (x_{H_2} = 0.167)	GERG-2004	0.71	13.92	578.6	57.6

Based on Table 2, adding hydrogen to the natural gas lowers the viscous resistance. The frictional pressure loss decreases and becomes more significant when the throughput increases.
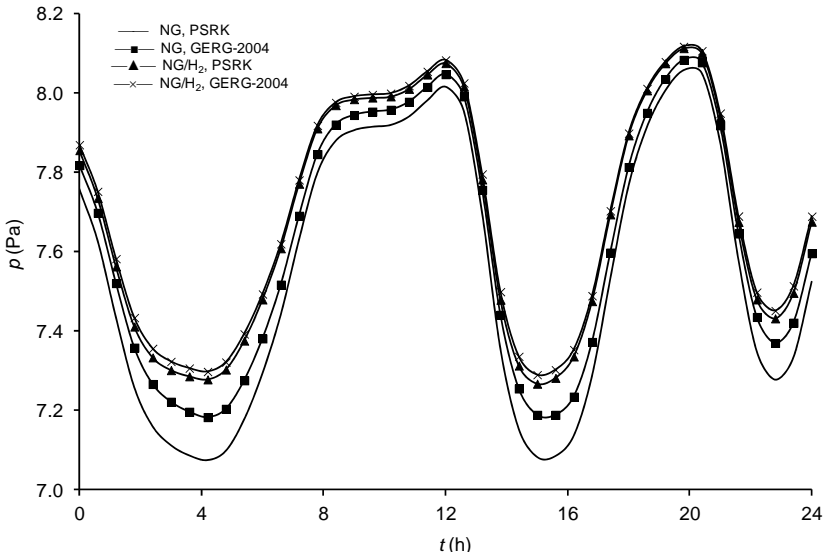
Fig. 4. Variation in pressure at the end of the pipeline, $x = L$
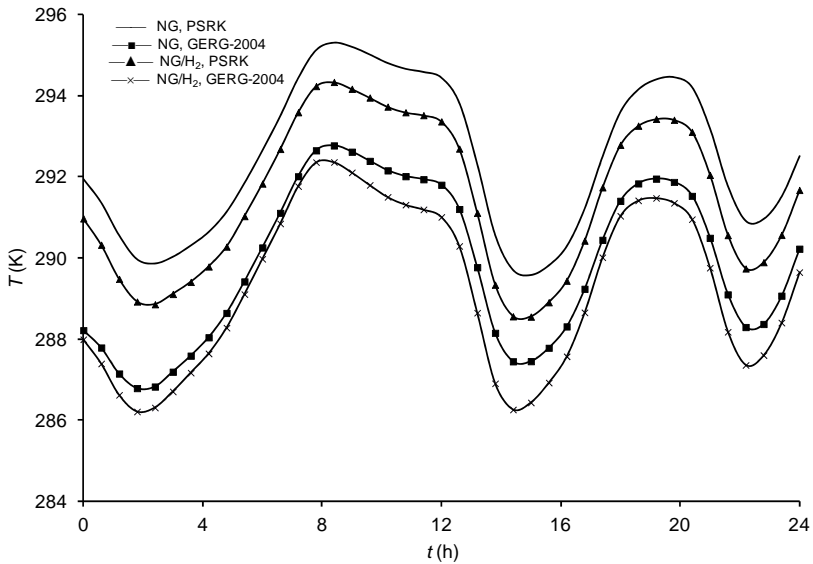
Fig. 5. Variation in temperature at the end of the pipeline, $x = L$

The Joule-Thomson effect dominates the temperature gradient because the temperature increases when hydrogen under expansion increases its temperature. Hence, the temperature gradient for the H_2/NG mixtures is lower.
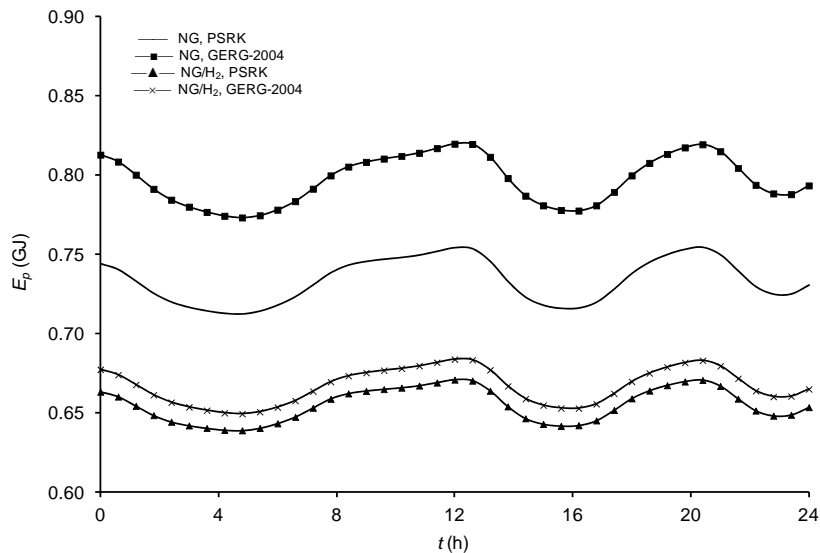
Fig. 6. Distribution of the linepack-energy in the pipeline

4. Conclusion

Two well-known equations of state are compared. The use of the GERG-2004 results in a higher pressure and lower temperature at the end of the pipeline in comparison with the PSRK method. This accounts for both natural gas and natural gas injected with hydrogen. The linepack-energy is estimated higher and the energy consumption lower by GERG-2004. The presence of hydrogen in natural gas mixture decreases the pressure and temperature gradient in the pipeline. The presence of hydrogen might cause problems to manage the supply and demand variations for short-term balancing periods due to the loss in linepack-energy. The compressor power decreases for the hydrogen-natural gas mixture.

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