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Mathematical Modeling of Non-Isothermal Multi-Component Fluid Flow in Pipes Applying to Rapid Gas Decompression in Rich and Base Gases

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Abstract**—**The paper presents a one-dimensional transient mathematical model of compressible non-isothermal multi-component fluid mixture flow in a pipe. The set of the mass, momentum and enthalpy conservation equations for gas phase is solved in the model. Thermo-physical properties of multi-component gas mixture are calculated by solving the Equation of State (EOS) model. The Soave-Redlich-Kwong (SRK-EOS) model is chosen. Gas mixture viscosity is calculated on the basis of the Lee-Gonzales-Eakin (LGE) correlation. Numerical analysis of rapid gas decompression process in rich and base natural gases is made on the basis of the proposed mathematical model. The model is successfully validated on the experimental data [1]. The proposed mathematical model shows a very good agreement with the experimental data [1] in a wide range of pressure values and predicts the decompression in rich and base gas mixtures much better than analytical and mathematical models, which are available from the open source literature.

Keywords**—**Mathematical model, Multi-Component gas mixture flow, Rapid Gas Decompression

I. INTRODUCTION

THE rupture on the pipeline wall brings numerous problems for oil and gas engineers. It cost a lot of money and time fixing the problem. The fracture propagation control in oil and gas transport pipeline service usually is made on the basis of the Battelle two-curve method, which was developed by the Battelle Columbus Laboratories in order to determine of the fracture arrest toughness [2,3]. The fracture propagation speed in the pipeline wall material and the decompression wave speed in gas mixtures are required to be employed in the Battelle analysis. The fracture propagation is arrested when the decompression wave speed in gas mixtures is quicker than the fracture propagation velocity in the pipeline wall material. Therefore, the information about the decompression wave speed in different gas mixtures is very important for the fracture propagation control and for the pipeline design.

The fluid mixture composition, pipeline inner diameter, pressure, and temperature significantly influence on the decompression wave speed. The decompression in natural gas mixtures is very rapid non-isothermal process. A transient mathematical model of compressible non-isothermal multi-component fluid mixture flow in pipes gives the information on the flow behavior correctly in a wide range of the operating parameters. The information on the mathematical modeling of rapid gas decompression process in natural gas mixtures is extremely limited in the open source literature. Very extensive experimental measurements of the decompression wave speed in rich and base natural gas mixtures were made last year's [1, 4-7]. The influence of the shock tube inner diameter, gas mixture composition, pressure, and temperature was carefully examined in details experimentally. Pressure values were varied in the range between 10 MPa and 37 MPa [1,6]. Most of measurements were made on the small-diameter shock tube, where the friction force influences on the flow behavior much stronger compare to large-diameter pipes.

The program GASDECOM [8], which is based on the analytical solution of the decompression wave speed determination, is used by oil and gas engineers in order to calculate the decompression wave speed values [1,5] as well. The program predicts decompression wave speed values with a reasonably good level of accuracy. However, those values are determined from the area of the shock tube, which is near to the rupture disc. The friction force is not accounted for in the analysis here. The comparison between measured data and GASDECOM calculations is very poor, when the gas decompression wave speed is determined from pressure transducers, which are located far away from the rupture end of the pipe, and where the friction influences on the flow behavior significantly. Analytical models do not take the friction force into consideration usually at all. Numerical simulations of the rapid gas decompression process in rich and base gas mixtures were performed [5] by using the commercial one-dimensional OLGA code (SPT-group) [9] as well. All predictions were made by using OLGA [5] show a poor comparison with experimental data and all calculated values were over-predicted.

The paper presents a one-dimensional transient mathematical model of compressible non-isothermal multi-component fluid mixture flow in a pipe. Numerical analysis of rapid gas decompression process in rich and base natural gases is made on the basis of the proposed mathematical model. The model is successfully validated on the experimental data [1] and it showed a very good agreement with this experimental data. The proposed mathematical model predicts the

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decompression wave speed in natural gas mixtures much better compare to other mathematical and analytical models, which are available from the open source literature nowadays.

II. MATHEMATICAL MODEL OF ONE-DIMENSIONAL TRANSIENT SINGLE-PHASE FLOW

The set of the mass, momentum and enthalpy conservation equations for the gas phase is solved in the mathematical model. This set of equations for the single phase gas mixture in general form is written as [10]:

$$\frac{\partial \alpha_G \rho_G}{\partial t} + \frac{\partial \alpha_G \rho_G U_G}{\partial z} = 0 \tag{1}$$

$$\frac{\partial \alpha_G \rho_G U_G}{\partial t} + \frac{\partial \alpha_G \rho_G U_G^2}{\partial z} = -\alpha_G \frac{\partial P}{\partial z} - R_{G-Wall} \tag{2}$$

$$\frac{\partial \alpha_G \rho_G h_G}{\partial t} + \frac{\partial \alpha_G \rho_G U_G h_G}{\partial z} = \alpha_G \left(\frac{\partial P}{\partial t} + U_G \frac{\partial P}{\partial z} \right) \tag{3}$$

Here, α_G is the volume fraction of the gas mixture; ρ_G is the density of the gas mixture; U_G is the velocity of the gas mixture; *P* is the total pressure; R_{G-Wall} is the friction term, h_G is the enthalpy of the fluid, t is the time, *z* is the axial co-ordinate. The friction term is written as [11]:

$$\begin{gathered} -R_{G-Wall} = -\frac{\Pi}{S} \tau_{G-Wall}, \tau_{G-Wall} = \frac{\xi_{G-Wall} \rho_G U_G^2}{8}, \\ \begin{cases} \xi_{G-Wall} = 64 / Re_G & , \quad Re_G < 1600 \\ \xi_{G-Wall} = 0.316 / Re_G^{0.25} & , \quad Re_G > 1600 \end{cases} \end{gathered} \tag{4}$$

Here, Π is the perimeter of the pipe; *S* is the cross-sectional area of the pipe; τ_{G-Wall} is the friction term (i.e. Gas-Wall interaction); ξ_{G-Wall} is the friction coefficient. The dimensionless complex is written as follows:

$$Re_G = \rho_G U_G D_{pipe} / \mu_G \tag{5}$$

Here, D_{pipe} is the diameter of the pipe; μ_G is the viscosity of the fluid.

III. THERMO-PHYSICAL PROPERTIES OF GAS MIXTURE

Thermo-physical fluid properties are modeled by solving of the Equation of State (EOS) in the form of the Soave-Redlich-Kwong model [12]. The set of equations and correlations (SRK-EOS) may be written as [12]:

$$P = \frac{RT}{(V-b)} - \frac{a}{V(V+b)} \tag{6}$$

$$a = \sum_{i=1}^{N} \sum_{j=1}^{N} z_i z_j \sqrt{a_i a_j} \left(1 - k_{ij}\right), b = \sum_{i=1}^{N} z_i b_i \tag{7}$$

$$\begin{gathered} a_i = 0.42748 \frac{R^2 T_{Ci}^2}{P_{Ci}} \left[1 + m_i \left(1 - \sqrt{\frac{T}{T_{Ci}}} \right) \right]^2, \\ b_i = 0.08664 \frac{R T_{Ci}}{P_{Ci}} \end{gathered} \tag{8}$$

$$m_i = 0.48 + 1.574\, \omega_i - 0.176\, \omega_i^2 \tag{9}$$

Here, *V* is the volume of the gas mixture; *N* is the number of components in the gas mixture; *T* is the temperature of the gas mixture; *R* is the universal gas constant; ω_i is the acentric factor of the component *i*; P_{Ci}, T_{Ci} are critical values of the pressure and temperature, correspondently; z_i is the mole fraction of the component *i*. The compressibility factor (*Z*) of the gas mixture is calculated from the following equation [12]:

$$Z^3 - Z^2 + \left(A - B - B^2\right) Z - AB = 0 \tag{10}$$

$$A = \frac{aP}{R^2 T^2}, B = \frac{bP}{RT} \tag{11}$$

The viscosity of the gas mixture is calculated by using of the Lee-Gonzales-Eakin (LGE) correlation and may be written as [13]:

$$\mu_g = D_1 \cdot 10^{-4} \cdot exp\left(D_2\, \rho_g^{D_3}\right) \tag{12}$$

Where the parameters are calculated as [13]:

$$D_1 = \frac{\left(9.38 + 0.016\, MW_g\right) T^{1.5}}{209.2 + 19.26\, MW_g + T} \tag{13}$$

$$D_2 = 3.448 + \left(\frac{986.4}{T}\right) + 0.01 MW_g \tag{14}$$

$$D_3 = 2.447 - 0.224 \cdot D_2 \tag{15}$$

Here, MW_g is the molecular weight of the gas mixture, ρ_g is the gas density in (g/cc), T is the temperature in (*R*).

IV. NUMERICAL SCHEME AND ALGORITHM

The algorithm of solving of the set of One- Dimensional transient governing equations of the fluid mixture flow in a pipe is based on the Tri-Diagonal Matrix Algorithm (TDMA), also known as the Thomas algorithm [14]. It is a simplified form of Gaussian elimination that can be used to solve tri-diagonal systems of equations. The equation is transformed into the following discrete analog (tri-diagonal system) [14]:

$$a_i\, T_i = b_i\, T_{i+1} + c_i\, T_{i-1} + d_i \tag{16}$$

Where i = 1, N. Following correlation is the solution of the equation, which have to be solved:

$$T_i = P_i\, T_{i+1} + Q_i \tag{17}$$

Here, the coefficients may be found from the following correlations:

$$P_i = \frac{b_i}{a_i - c_i\, P_{i-1}}, Q_i = \frac{d_i + c_i\, Q_{i-1}}{a_i - c_i\, P_{i-1}} \tag{18}$$

Following algorithm should be performed in order to solve the equations [14]:

a) P_1 and Q_1 is calculated from (18) assuming $c_1 = 0$.

b) P_1 and Q_1 is calculated from (18) where *i=2,…,N.*

c) Assume the following $T_N = Q_N$.

d) T_i are calculated from (17) where $i=(N-1),\dots,1$.

TDMA algorithm is a convenient equation solver if the algebraic equation can be represented in the form of (16). Unsteady equations have to be solved by using the same scheme, which was described above. The set of unsteady governing equations is transformed into the form of (16) by using the fully implicit numerical scheme. In this case the equation is reduces to the steady state discretization equation if the time step goes to infinity.

V. GAS DECOMPRESSION PROGRAM

A one-dimensional transient mathematical model of compressible non-isothermal multi-component fluid mixture flow in a pipe was developed under the research project in PETROSOFT D&C. The set of the mass, momentum and enthalpy conservation equations for gas phase is solved in the model. Thermo-physical properties of multi-component gas mixture are calculated by solving the Equation of State (EOS) model. The Soave-Redlich-Kwong (SRK-EOS) model is chosen. Gas mixture viscosity is calculated on the basis of the Lee-Gonzales-Eakin (LGE) correlation. The mathematical model was implemented into the FORTRAN computer code and was named the “Gas Decompression Program” (GDP code). More information about the GDP code is available on www.petrosoft-dc.com.

VI. NUMERICAL ANALYSIS OF RAPID GAS DECOMPRESSION IN BASE NATURAL GAS MIXTURES

The proposed mathematical model was validated on the experimental data on rapid gas decompression in base natural gas mixture [1]. Experimental measurements were conducted by TCPL (Trans Canada Pipe Lines) at TCPL Gas Dynamic Test Facility in Didsbury, Alberta, Canada [1]. The decompression test facility was constructed by TCPL having the following options [1]:

- Maximum values of the initial pressure of up to 22 MPa;
- Low initial temperature values, which are down up to $-20^o C$
- Flexibility in natural gas compositions having the methane fraction (C1) in the range of 70-95%.

The main test section of the facility is the shock tube, which is 30 meters long. The inner pipe diameter is 49.325 mm. The internal surface of the tube has a roughness, which is better than 40 micro-inches. A rupture disc is placed at one end of the pipe, which is upon rupturing. A decompression wave propagates up into the pressurized test section. A few high frequency responses Pressure Transducers (PT) are mounted into the tube in order to capture the time history of the expansion fan [1]. Several rupture discs were introduced into the shock tube end for different pressures at rupture. The initial temperature was dependent on the ambient atmospheric conditions. Decompression wave speed values were determined from the time between signals from P1 and P8 pressure transducers as well as the time between signals from P5 and P6 transducers.

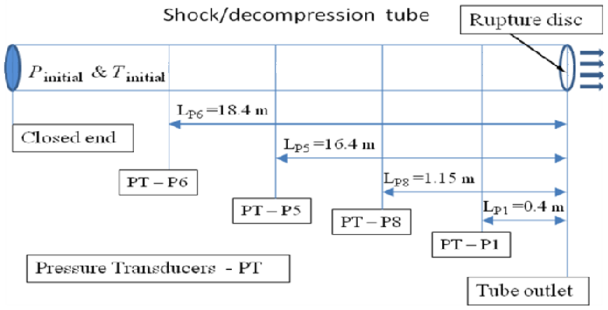


Fig. 1 Schematic of the experimental decompression tube

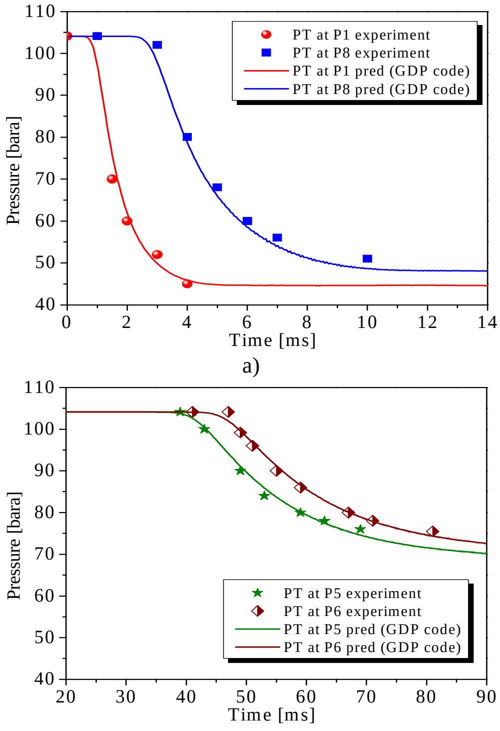
Fig. 1 shows the schematic view of the experimental decompression tube. Despite the fact that the main test section of the shock tube is 30 meters long, the decompression pipe having a length of 50 meters is simulated from the point of view of the numerical stability of results. The inner pipe diameter is 49.325 mm. One end of the shock tube is selected to be the closed end. The rupture disc is introduced into other end of the pipe. Distances between the rupture disc and pressure transducers are selected to be identical to real distances on the experimental decompression tube as it shown on Fig. 1.

Those distances between pressure transducers P1, P8, P5, P6 and the rupture disc are 0.4, 1.15, 16.4, 18.4 meters, correspondently. Three cases having a different initial pressure values are considered (table 1) to simulate. The temperature and gas mixture composition are different in each case as well. The initial pressure ($P_{initial}$) in the shock tube before rupture started is set up to 10.41 MPa, 13.8 MPa and 20.67 MPa. The initial temperature ($T_{initial}$) in the decompression pipe is set up to 274.07 K, 264.77 K and 264.72 K, correspondently. The following gas mixture composition (base natural gas), initial pressure and initial temperature were selected (table 1):

TABLE I
GAS COMPOSITION (MOLE %), INITIAL PRESSURE (MPA) AND TEMPERATURE (K)

	Case 1	Case 2	Case3
$P_{initial}$	10.41	13.8	20.67
$T_{initial}$	274.07	264.77	264.72
N2	0.697	0.647	0.699
CO2	1.097	1.197	1.279
C1	92.955	93.02	92.757
C2	4.076	3.876	4.075
C3	0.8	0.909	0.861
i-C4	0.099	0.108	0.103
n-C4	0.137	0.158	0.146
i-C5	0.066	0.059	0.053
n-C5	0.073	0.026	0.027

Simulations of those three test cases are made by using the proposed mathematical model. The decompression process in base natural gas mixtures having the inlet and boundary condition identical to the experimental one is simulated. Predictions are started with the initial pressure of 10.41 MPa in each computational cell of the pipe (case 1). New values of the velocity, temperature, density and pressure are calculated at each time step. It is chosen to be large enough until a value where the convergence of the set of governing equations is not reached and the calculations are not stable.

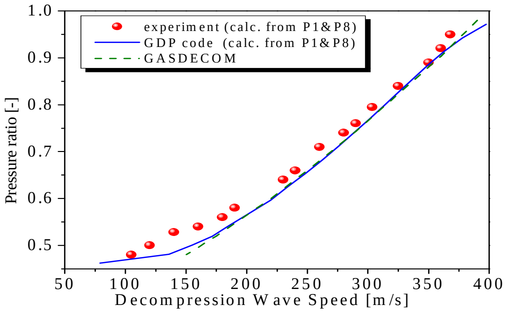


a)

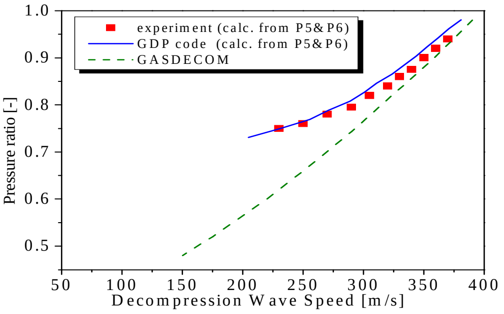
b)

Fig. 2 Pressure time history at PT-P1&P8 (a) and PT-P5&P6 (b) case 1

Pressure values are collected at PT locations P1, P8, P5 and P6 at each time step started from the beginning. Fig. 2 shows the evolution of pressure values at PT-P1&P8 (fig. 2(a)) and PT-P5&P6 (fig. 2(b)) locations for the case 1. Fig. 3 shows the decompression wave speed, which was determined from PT-P1&P8 (fig. 3(a)) and P5&P6 (fig. 3(b)), correspondently. Pressure values are normalized on the initial pressure before rupturing. Experimental points are shown in all figures as symbols. Continues lines represent predictions using proposed GDP code. All calculations of the decompression wave speed by using analytical GASDECOM [8] were made by [1] having the same gas composition, initial pressure and temperate (i.e. case1, case 2 and case 3). Those analytical data were taken from [1] in order to compare those predictions with GDP calculations (fig. 3, 5, 7). Broken curves represent GASDECOM numerical results [1] here in all figures.



a)

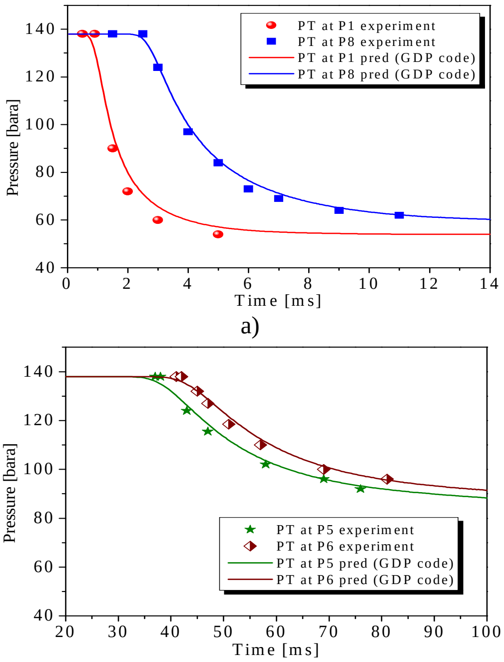


b)

Fig. 3 Decompression wave speed as a function of pressure ratio

Both Fig. 2 and 3 shows a good agreement between experimental data and predictions were made by using the GDP code. The proposed model predicts the decompression wave speed, which is determined from PT locations P5 and P6, much better than the analytical GASDECOMP.

Other predictions of the decompression wave speed values are made by using the same shock tube topology (Fig. 1), but having higher initial pressure before rupturing (case 2).

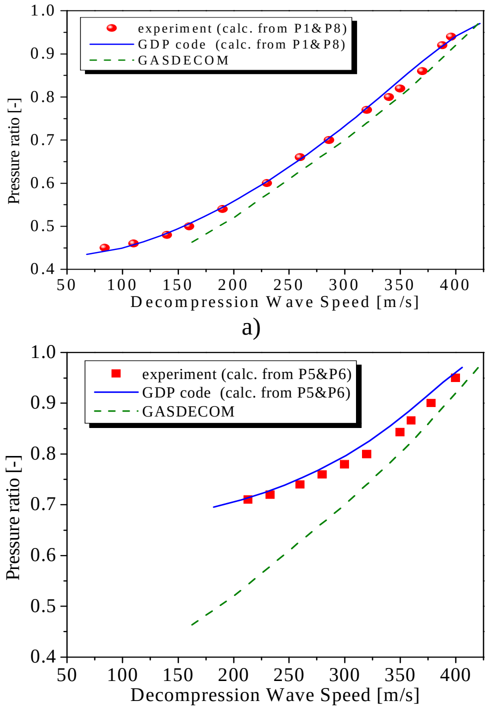


a)

b)

Fig. 4 Pressure time history at PT-P1&P8 (a) and PT-P5&P6 (b) case 2

The initial temperature and gas composition were up-dated according to the case 1 (table 1) as well. Pressure evolution values show a reasonably good agreement with experimental data (fig. 4). The prediction, which was made by using GDP code, shows a better agreement with experimental data compare to another simulation [1], which was performed by using the analytical GASDECOM model (Fig. 5).

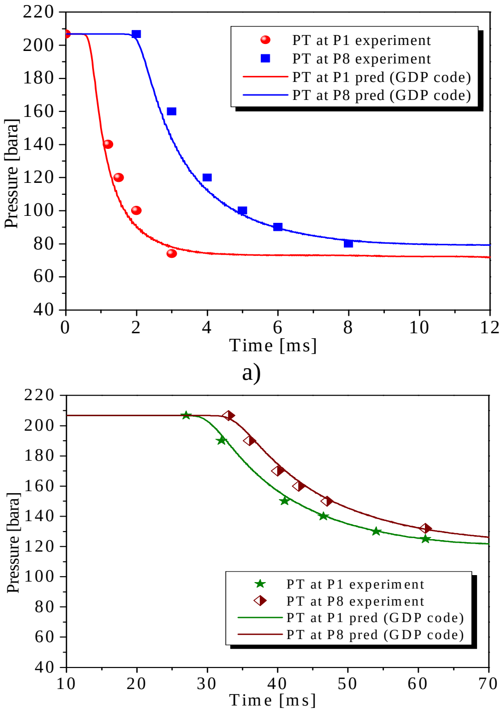


a)

b)

Fig. 5 Decompression wave speed as a function of pressure ratio

The decompression wave speed is determined from pressure transducers, which are located far away from the rupture end of the pipe (i.e. P5 and P6), shows a very good comparison between the proposed model and experiments.



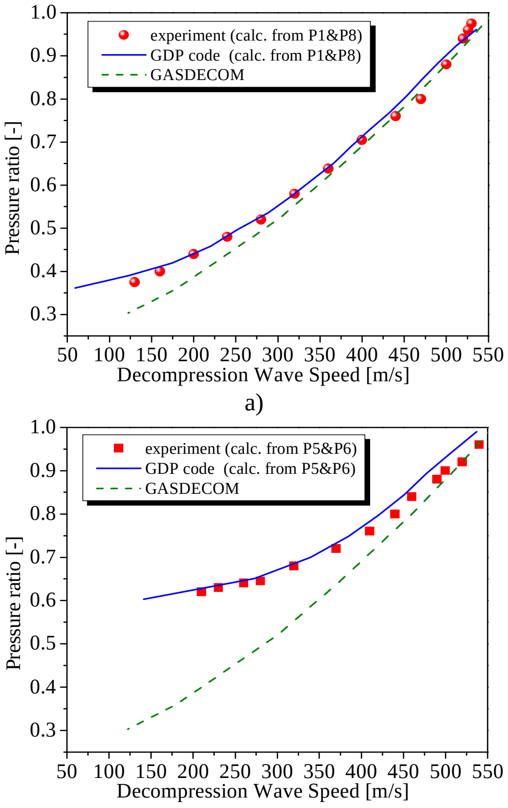
a)

b)

Fig. 6 Pressure time history at PT-P1&P8 (a) and PT-P5&P6 (b) case 3

Last predictions of the decompression wave speed were made again for the same shock tube (fig. 1) but having the highest initial pressure value from all three cases (table 1, case 3). The initial temperature and gas composition before rupturing were almost identical to previous case (table 1). The agreement between predicted values of the pressure time evolution and experiments has a high order of magnitude (fig. 6).

The prediction, which was made by using the proposed model, shows a much better agreement with experimental data compare to the analytical model (fig. 7). The decompression wave speed determined from P5 and P6 pressure transducers shows a very good comparison between the proposed model and experiments as well.



a)

b)

Fig. 7 Decompression wave speed as a function of pressure ratio

Analytical gas decompression model GASDECOM [8] is one of the most commonly used engineering software in oil and gas field applications in order to perform quick simulations of the decompression wave speed in natural gases. However, this model does not account for the friction between the gas mixture and pipe wall. The friction does not contribute a lot into the total force balance in the area, which is close to the rupture disc. Hence, the flow behavior is changed significantly in the area of the pipe, which is far away from the rapture place. It was observed experimentally that the decompression wave speed, which is calculated from pressure transducers P5 and P6, father away from the rupture end is much lower than the corresponding one (fig. 3,5,7), which is determined from a closer pair of P1 and P8 [1]. Therefore, the analytical GASDECOM does not simulate the decompression process in natural gas mixtures correctly in the case of small-diameter tubes. Values are over-predicted in this case.

Simulations of rapid gas decompression process in rich and base gas mixtures were made [5] by using well-know commercial 1D software OLGA developed by SPT-group [9]. All predictions were made by OLGA [1] are not in good agreement with the experimental data. The calculation of pressure evolution values showed that OLGA's predictions of the frontal wave speed are significantly lower than measurements [5].

Therefore, the proposed mathematical model of transient compressible non-isothermal multi-component gas mixture flow in a pipe predicts the decompression process in base natural gases much better than other analytical and mathematical models, which are available from the open source literature. Moreover, simulations, which are made by using the presented mathematical model, are quick in time and allow simulating of large-scale pipes and shock tubes having a few meters or kilometers in length.

VII. CONCLUSION

A one-dimensional transient mathematical model of compressible non-isothermal multi-component fluid mixture flow in a pipe is presented in the paper. The set of the mass, momentum and enthalpy conservation equations for gas phase is solved in the model. Thermo-physical properties of multi-component gas mixture are calculated by solving the Equation of State (EOS) model. The Soave-Redlich-Kwong (SRK-EOS) model is chosen. Gas mixture viscosity is calculated on the basis of the Lee-Gonzales-Eakin (LGE) correlation.

Numerical analysis of rapid gas decompression process in rich and base natural gases, which was made by using of the proposed mathematical model, is presented in the paper. The model is successfully validated on the experimental data [1]. The proposed mathematical model showed a very good agreement with this experimental data [1] in a wide range of pressure values and natural gas compositions. Paper showed that the mathematical model predicts the decompression in rich and base gas mixtures much better than the analytical and mathematical models, which are available from the open source literature nowadays.

The presented model is highly necessary and useful in the pipeline designing and in the flow assurance investigation. The minimum of fracture arrest toughness of the pipe wall material may be determined on the basis of the Battelle two-curve method with taking into account of the proposed model together with fracture propagation speed model. The influence of temperature, pressure, fluid composition, and pipeline diameter is quickly examined by using of the presented mathematical model.

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