International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:6, No:1, 2012

Numerical Analysis of Rapid Gas Decompression in Pure Nitrogen using 1D and 3D Transient Mathematical Models of Gas Flow in Pipes

Evgeniy Burlutskiy

Abstract**—**The paper presents a numerical investigation on the rapid gas decompression in pure nitrogen which is made by using the one-dimensional (1D) and three-dimensional (3D) mathematical models of transient compressible non-isothermal fluid flow in pipes. A 1D transient mathematical model of compressible thermal multi-component fluid mixture flow in pipes is presented. 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. This model is successfully validated on the experimental data [1] and shows a good agreement with measurements. A 3D transient mathematical model of compressible thermal single-component gas flow in pipes, which is built by using the CFD Fluent code (ANSYS), is presented in the paper. The set of unsteady Reynolds-averaged conservation equations for gas phase is solved. Thermo-physical properties of single-component gas are calculated by solving the Real Gas Equation of State (EOS) model. The simplest case of gas decompression in pure nitrogen is simulated using both 1D and 3D models. The ability of both models to simulate the process of rapid decompression with a high order of agreement with each other is tested. Both, 1D and 3D numerical results show a good agreement between each other. The numerical investigation shows that 3D CFD model is very helpful in order to validate 1D simulation results if the experimental data is absent or limited.

Keywords**—**Mathematical model, Rapid Gas Decompression

I. INTRODUCTION

THE fracture propagation control is usually made on the basis of the Battelle two-curve method, which was developed by the Battelle Columbus Laboratories [2,3]). This method helps to determine the fracture arrest toughness when a pipeline is ruptured. The fracture propagation speed in a pipeline wall and the decompression wave speed in gas mixtures are required to be used 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 a pipeline wall material. Therefore, the accuracy in the calculation of the decompression wave speed in gas mixtures is very important in fracture propagation control analysis.

The decompression process in natural gas mixtures is very rapid non-isothermal process. A transient mathematical model of compressible thermal multi-component fluid mixture flow in pipes helps to study the flow behavior in a wide range of the operating parameters. Extensive experimental measurements of the decompression wave speed in rich and base natural gas mixtures were made last years [1, 4-7]. The influence of shock tube inner diameter, gas mixture composition, pressure, and temperature was carefully examined in details experimentally. Most of measurements were made on a small-diameter shock tube, where the friction force influences on the flow behavior much stronger compare to large-diameter pipes. However, the information on the decompression wave speed measurements is extremely limited in the open source literature. Papers on the experimental measurements of the gas decompression in carbon dioxide mixtures are absent in the open source literature too.

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 the decompression wave speed values with a reasonably good level of accuracy. However, 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.

The paper presents a numerical investigation on the rapid gas decompression in pure nitrogen which is made by using 1D and 3D mathematical models of transient compressible thermal fluid flow in pipes. A 1D mathematical model of compressible thermal multi-component fluid mixture flow in a pipe is presented. The model is validated [9,10] on the experimental data [1] and shows a good agreement with those measurements. A 3D mathematical model of compressible thermal single-component gas flow in pipes, which is built by using the CFD Fluent code (ANSYS), is presented in the paper. The simulation of rapid gas decompression in pure nitrogen is made by using the 3D model and results of calculation are compared with 1D prediction. The ability of both models to simulate the decompression process with a

Dr. Evgeniy Burlutskiy was with PETROSOFT D&C 208511 Singapore. He is now with the A*STAR Institute of High Performance Computing (IHPC), 1 Fusionopolis Way, 138632, Singapore (phone: +65 6419 1386; e-mail: burlutskiye@ihpc.a-star.edu.sg and e.burlutskiy@petrosoft-dc.com).

high order of agreement between each other is tested on the simple gas flow case. Both, 1D and 3D numerical results show a very good agreement between each other.

II. ONE-DIMENSIONAL MATHEMATICAL MODEL OF 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 [11]:

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

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

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

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 coordinate. The friction term is written as [12]:

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

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

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

III. THERMO-PHYSICAL PROPERTIES OF GAS MIXTURE IN ONE-DIMENSIONAL MATHEMATICAL MODEL

Thermo-physical fluid properties are modeled by solving of the Equation of State (EOS) in the form of the Soave-Redlich-Kwong model [13]. The set of equations and correlations (SRK-EOS) may be written as [13]:

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

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

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

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

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 [13]:

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

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

The viscosity of gas mixture is calculated by using of the Lee-Gonzales-Eakin (LGE) correlation [14]. 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 [15]. It is a simplified form of Gaussian elimination that can be used to solve tri-diagonal systems of equations. The set of unsteady governing equations is transformed into the standard form of the discrete analog of the tri-diagonal system [15] 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.

IV. GAS DECOMPRESSION PROGRAM

A one-dimensional transient mathematical model of compressible thermal multi-component fluid mixture flow in a pipe was developed under the research project “Multi-component Gas mixture flows in pipelines and wells” in PETROSOFT D&C. This 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.

V. THREE-DIMENSIONAL MATHEMATICAL MODEL OF TRANSIENT SINGLE-PHASE FLOW USING THE FLUENT CODE (ANSYS)

Transient simulations of rapid gas decompression in pure nitrogen are performed by using the CFD Fluent code (ANSYS). The unsteady Reynolds-averaged conservation equations are solved in order to simulate the Eulerian fluid flow field. For unsteady flow case, the set of governing equations is written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0 \tag{12}$$

$$\frac{\partial}{\partial t}\left(\rho u_j\right) + \frac{\partial}{\partial x_j}\left(\rho u_j u_i - \tau_{ij}\right) = -\frac{\partial p}{\partial x_i} \tag{13}$$

Where, x_i is the Cartesian coordinate (*i*= 1, 2, 3), u_i is the absolute fluid velocity component in direction (x_i), p is the pressure, ρ is the fluid density, and τ_{ij} is the stress tensor component. For the turbulent flow case, the stress tensor is written as:

$$\tau_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} - \bar{\rho}\overline{u_i' u_j'} \qquad (14)$$

Here, S_{ij} is the rate of strain tensor, μ is the molecular dynamic viscosity of the fluid, δ_{ij} is the “Kronecker delta” function (which is unity when $i = j$ and zero otherwise), and $\overline{u_i' u_j'}$ are the fluctuations of the fluid velocity as a result of the Reynolds averaging procedure. These fluctuations represent the additional Reynolds stress due to the turbulent motion. In order to model the turbulent structure of the fluid phase, the $\overline{u_i' u_j'}$ component is determined using the Boussinesq hypothesis. The conservation equations are closed using the Realizable k-ε turbulence model, which is used together with the enhanced wall function treatment for modeling boundary conditions at the wall.

VI. EXPERIMENTAL VALIDATION OF 1D GDP CODE ON RAPID DECOMPRESSION IN NATURAL GAS MIXTURES

The presented mathematical model was successfully validated [9, 10] on the experimental data on the rapid gas decompression in base natural gas mixtures [1]. Those experimental measurements were conducted by TCPL (Trans Canada Pipe Lines) at TCPL Gas Dynamic Test Facility in Didsbury, Alberta, Canada [1]. 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]. Decompression wave speed values were determined from the time between signals from PT-P1 and PT-P8 as well as from PT-P5 and PT-P6 (fig. 1). Fig. 1 shows the schematic of the experimental decompression tube. The computational decompression pipe has a length of 50 meters long. 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 shown on fig. 1.

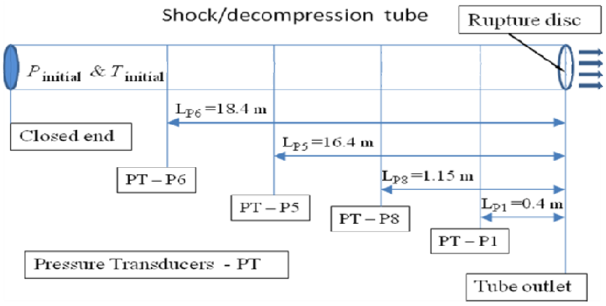


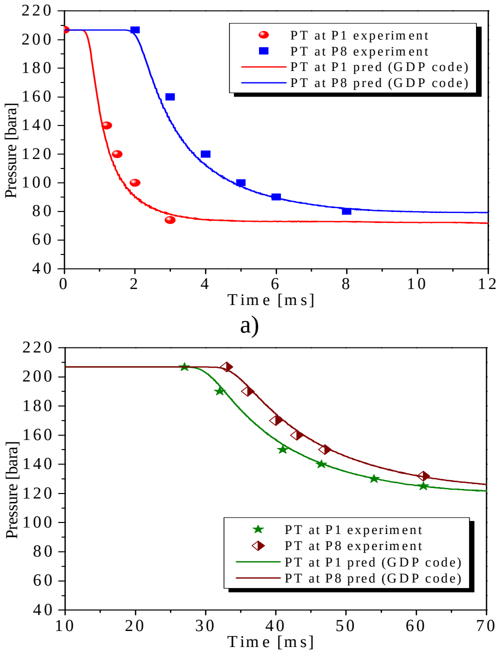
Fig. 1 Schematic of the experimental decompression tube

Three different experimental cases having a different gas composition, initial pressure, and temperature values are simulated using the GDP code [9, 10]. Simulation results of one test case (Table I) are shown. The following gas mixture composition, initial pressure and initial temperature were used to perform the simulation (Table I):

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

	Case 1
$P_{initial}$	20.67
$T_{initial}$	264.72
N2	0.699
CO2	1.279
C1	92.757
C2	4.075
C3	0.861
i-C4	0.103
n-C4	0.146
i-C5	0.053
n-C5	0.027

Rapid gas decompression in base natural gas mixtures having the inlet and boundary conditions (Table I), which are identical to the experimental one, is simulated by using the presented mathematical model. Predictions are started with the initial pressure of 20.67 MPa in each computational cell of the pipe. New values of the velocity, temperature, density and pressure are calculated after each time step. The upper limit of the time step was selected from the point of view of the numerical stability. Pressure values were collected at PT locations P1, P8, P5 and P6 after each time step started from the beginning. Fig. 2 shows the evolution of pressure values at P1&P8 (fig. 2(a)) and P5&P6 (fig. 2(b)) PT locations.

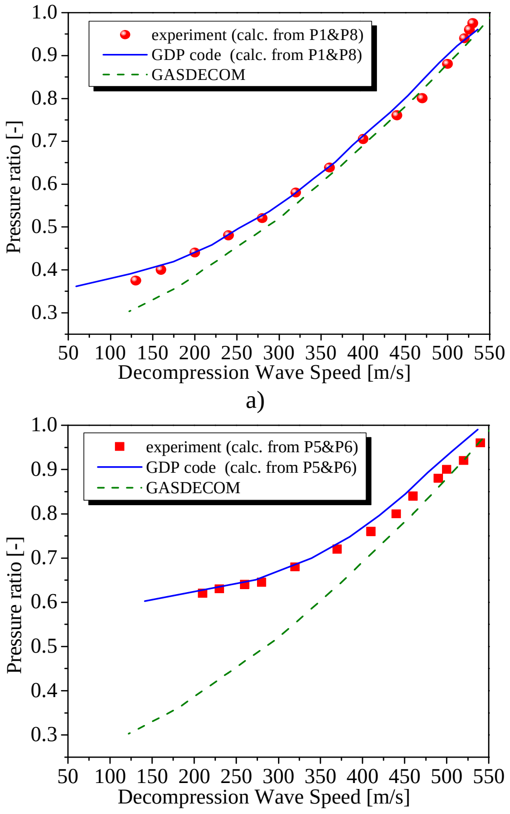


a)

b)

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

Fig. 3 shows the decompression wave speed, which was determined from P1&P8 (fig. 3(a)) and P5&P6 (fig. 3(b)) locations, correspondently. Pressure values are normalized on the initial pressure before rupturing. Experimental points are shown in all figures as symbols. Continues lines represent predictions, which are made by using the proposed GDP code. Calculations of the decompression wave speed by using analytical GASDECOM [8] are made by [1] setting up the same gas composition, initial pressure and temperate (i.e. case1).



a)

b)

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

Those analytical data are taken from [1] in order to compare those predictions with the GDP calculations (fig. 3). Broken curves represent GASDECOM numerical results [1]. All predictions on the time evolution of pressure values at different PT locations, which are performed by using the GDP model, are in good agreement with the experimental data. The presented 1D model predicts the decompression wave speed, which is determined from P5 and P6 PT locations, much better than the analytical GASDECOMP.

The analytical gas decompression model GASDECOM [8] is one of the most commonly used engineering software in oil and gas field applications. However, the friction between the gas and the pipe wall is not accounted for in the model. This fact is significantly limited the application of GASDECOM to the decompression wave calculation. The presented 1D mathematical model of transient compressible thermal multi-component gas mixture flow in pipes predicts the decompression process in base natural gases much better than other analytical and mathematical models, which are available from the open source literature. However, experimental data on the rapid gas decompression process in gases are limited. Therefore, the paper proposes to use 3D CFD model as a validation tool for 1D model calculations when experimental measurements are absent. The idea to conduct a numerical study of a simple gas flow in a pipe by using of 1D and 3D models is tested here.

VII. Numerical Analysis Of Rapid Gas Decompression In Pure Nitrogen Using 1D And 3D Models

The numerical analysis of rapid gas decompression in pure nitrogen using 1D and 3D models is performed. The comparison of both predicted results will show the ability of both approaches (1D and 3D) on successful simulation of simple flows with a high level of agreement between each other. It will give the additional confidence in 1D simulation in cases when experimental measurements are absent or limited.

The same decompression tube (Table I) is selected for simulations using both 1D and 3D codes. The prediction of the decompression flow starts from no-flow stagnant conditions in the pipe. The initial pressure is 10 MPa. The initial temperature is 260 K. The PT locations (PT-1, 2, 3, 4) for the case of pure nitrogen simulation are differed compare to the previous case (fig. 4). All PT are located near the rupture end of the pipe. The flow through the rupture disc begins after when rupturing is started.

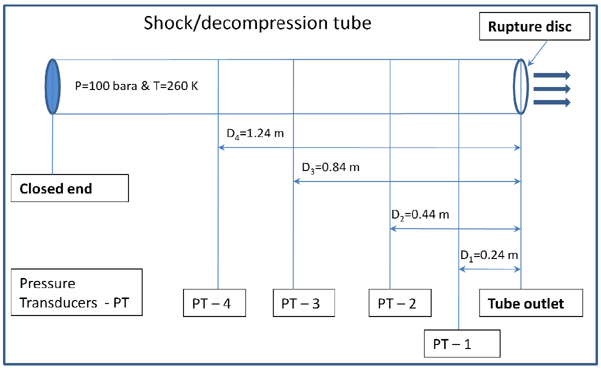
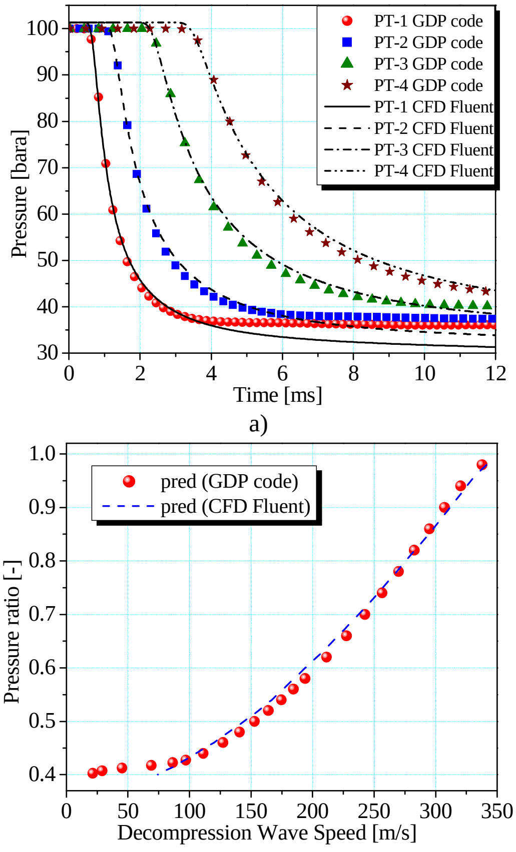


Fig. 4 Schematic of the decompression tube

Basic simulations of the decompression process in pure nitrogen by using CFD Fluent code (ANSYS) are performed on the computational domain having totally 300,000 computational cells. The length of the computational pipe is 10 meters long. A mesh refinement study was performed. Simulations, which are made on the refined computational mesh show grid independence compare to predictions, which are performed on the basic computational mesh. Predictions of the decompression in pure nitrogen are performed with different time steps too. Time step refinement study shows the time-step independence of the results starting from the time step, which is equal to 10^{-5} seconds. Most of simulations are made with the time step equal to 10^{-5} seconds. The real gas Redlich-Kwong (RK-EOS) model is chosen for predictions.

Predictions, which are made using 1D GDP code, are shown as symbols in fig. 5. Continues and broken lines represent calculations, which are performed by using 3D CFD model.



a)

b)

Fig. 5 Predicted pressure time history at different PT locations (a) and decompression wave speed as a function of pressure ratio (b)

Predicted values of the pressure time evolution at four different PT locations are shown in fig. 5(a). Calculations, which are performed by using the 1D GDP code and 3D CFD code, show a good agreement between each other for each PT location. The decompression wave speed is determined from PT-1 and PT-2 (fig. 4). The distribution of the decompression wave speed values in pure nitrogen is shown in fig. 5(b). Simulation results, which are performed by using 3D CFD code and 1D GDP code, are shown in figure both. Those numerical results are in a very good agreement with each other in a wide range of pressure values.

VIII. CONCLUSION

A numerical investigation of the rapid gas decompression in pure nitrogen, which is made by using the 1D and 3D transient mathematical models of compressible thermal fluid flow in pipes is performed. Results of this numerical study are presented in the paper.

A 1D mathematical model of compressible thermal multi-component fluid mixture flow in pipes is presented. 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 model validation on the experimental data [1] shows a good agreement with those measurements. Presented 1D mathematical model predicts the decompression in natural gas mixtures much better than the analytical GASDECOM. A commercial 3D transient mathematical model of compressible thermal single-component gas flow in pipes is presented in the paper too. The set of unsteady Reynolds-averaged conservation equations for the gas phase is solved. Thermo-physical properties of single-component gas are calculated by solving the Real Gas Equation of State (EOS) model.

The simplest case of the gas decompression in pure nitrogen is simulated using both 1D and 3D models. The ability of both models to simulate the process of the rapid decompression in pure nitrogen with a high order of agreement with each other is tested. Both 1D and 3D numerical results show a good agreement between each other. This numerical investigation shows that 3D CFD model is very helpful in order to validate 1D simulation results if the experimental data is absent or limited.

ACKNOWLEDGMENT

The author would like to acknowledge the financial support of PETROSOFT D&C to develop the presented mathematical model and to create the computer program (GDP code). The author would like to acknowledge the support of current employer A*STAR Institute of High Performance Computing (IHPC), Singapore for giving access to CFD Fluent code (ANSYS).

REFERENCES

[1] K.K. Botros, W. Studzinski, J. Geerligs, A. Glover, “Measurement of decompression wave speed in rich gas mixtures using a decompression tube,” *American Gas Association Proceedings –(AGA-2003)*, 2003.

[2] R.J. Eiber, T.A. Bubenik, W.A. Maxey, “Fracture control for natural gas pipelines,” *PRCI Report Number L51691*, 1993.

[3] R.J. Eiber, L. Carlson, B. Leis, “Fracture control requirements for gas transmission pipelines,” *Proceedings of the Fourth International Conference on Pipeline Technology*, p. 437, 2004.

[4] K.K. Botros, W. Studzinski, J. Geerligs, A. Glover, “Determination of decompression wave speed in rich gas mixtures,” *The Canadian Journal of Chemical Engineering*, vol. 82, pp. 880–891, 2004.

[5] K.K. Botros, J. Geerligs, J. Zhou, A. Glover, “Measurements of flow parameters and decompression wave speed follow rapture of rich gas pipelines, and comparison with GASDECOM,” *International Journal of Pressure Vessels and Piping*, vol. 84, pp. 358–367, 2007.

[6] K.K. Botros, J. Geerligs, R.J. Eiber, “Measurement of decompression wave speed in rich gas mixtures at high pressures (370 bars) using a specialized rupture tube,” *Journal of Pressure Vessel Technology*, vol. 132, 051303-15, 2010.

[7] K.K. Botros, J. Geerligs, B. Rothwell, L. Carlson, L. Fletcher, P. Venton, “Transferability of decompression wave speed measured by a small-diameter shock tube to full size pipelines and implications for determining required fracture propagation resistance,” *International Journal of Pressure Vessels and Piping*, vol. 87, pp. 681–695, 2010.

[8] GADECOM, Computer code for the calculation of gas decompression speed that is included in “*Fracture Control Technology for Natural Gas*

Pipelines", by R.J. Eiber, T.A. Bubenik, W.A. Maxey, *NG-18 report 208, AGA Catalog N L51691*, 1993.

[9] E. Burlutskiy, "Mathematical model of compressible non-isothermal flow of multi-component natural gas mixture in a pipe," *International Scientific Conference on Mechanics, S-Petersburg, Russia, January 2012,* to be published

[10] E. Burlutskiy, "Mathematical modelling of non-isothermal multi-component fluid flow in pipes applying to rapid gas decompression in rich and base natural gases," *International Conference on Fluid Mechanics, Heat Transfer and Thermodynamics –ICFMHTT-2012 (15-17 Jan 2012), Zurich, Switzerland,* to be published

[11] G.B. Wallis, "One-dimensional two-phase flows," *McGraw Hill, New York*, 1969.

[12] P.R.H. Blasius, "Das Aehnlichkeitsgesetz bei Reibungsvorgangen in Fluessigkeiten," *Forschungsheft*, vol. 131, pp. 1–41, 1913.

[13] G. Soave, "Equilibrium constants from a modified Redlich-Kwong equation of state," *Chemical Engineering Science,* vol. 27, pp. 1197-1203, 1979.

[14] A.L. Lee, M.N. Gonzales, B.E. Eakin, "The viscosity of natural gases," *Journal of Petroleum Technology,* pp. 997-1000, 2010.

[15] S. Patankar, "Numerical heat transfer and fluid flow," *Hemisphere Publishing, New York,* 1980.