



## ABSTRACT

The simulation of Hydrogen Compress Natural Gas HCNG was carried out using PDEtoolbox in which the boundary conditions are treated numerically. Transient flow of hydrogen compressed natural gas mixture requires accurate on the prediction of flow parameters. From Graphic User Interface (GUI) MATLAB there is window for boundary default values and b are exported into M-file for computation. In the proposed method solution domain, boundary condition and governing equation nonlinear systems of partial differential equations are specified. The result obtained

# SIMULATION OF HIGH PRESSURE TRANSIENT FLOW OF HYDROGEN NATURAL GAS FLOW IN PIPELINE USING MATLAB PDETOOL BOX

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## Introduction

Various stakeholders have made effort in realizing the replacement of hydrogen as world energy source. Natural gas are replace as fuels for engines, many researches are conducted on possibility of achieving this globally. The mixture of hydrogen with natural gas is starting point toward full fledge hydrogen usage as energy source (Haeseldonckx and D'haeseleer, 2011). Hydrogen natural mixture can be used in engine and turbines since hydrogen is also a flammable gas (Cheng R et al., 2009, Tabkhi F et al., 2008).

The benefit of hydrogen natural gas mixture are numerous, that includes the reduction of greenhouse gas level (Yang and Ogden, 2007). The low burning capacity of natural gas with oor storage ability of hydrogen will be over come if the two gases are mixed. The problem of high emission when leakage occur of natural gas will be taken care.

With the increasing rate of global warming due to carbon emission from energy source there is need for alternative source. World energy continuously increases which is expected to rich 60% of 2005 by 2030. The present energy source is mostly from fossil fuel therefore there is need of less or non-carbon emission source. In 19<sup>th</sup> century coal dominate energy source which was followed by petroleum oil, natural gas and nuclear energy takes over in 20<sup>th</sup> and 21<sup>st</sup> centuries. There is clear indication that hydrogen will possible taking over before the end of 21st century due to recent development (Winter, 2009). Due to research on possible replacement of fossil fuel sources of energy toward saving the greenhouse gas.



demonstrated a lot of accuracy and computational efficiency when compared with previous published result on several problems of HCNG transient flow.

Natural gas is one of energy source with less emission but high carbon emission when leakage occurs. It also has low burning capacity. There is need to overcoming these problems associated to natural gas for effective performance and reduction in carbon emission eventually if leakage occurs.

Hydrogen been the lightest and most abundant flammable gas in the universe is receiving global attention as an alternative energy source. It has high burning capacity but poor storage.(Elaoud and Hadj-Tai"eb, 2008). In an attempt towards realizing hydrogen economy, natural gas are enriched with hydrogen as a starting point (Baufume et al., 2011, Mohammadi et al., 2012)

To address problem of low burning capacity associated with natural gas and poor storage capacity of hydrogen, researches are conducted for possibility of mixing the two gases. Hence natural gas is enriched by adding some percentage of hydrogen, to obtain hydrogen compressed natural gas mixture (HCNG). HCNG needs to be transported to consumption point and the easiest way is through pipeline.

The transportation of gas is normally at unsteady state due to rapid closure of valves in meeting customer demand. To reduce production cost the existing natural gas pipeline network is normally used consequently there is need for proper analysis of HCNG transportation. HCNG will also serve as a testing ground toward free emission energy source by 2030.

Different types of models and numerical method are previously presented amid at improving accuracy and reduce computational cost; some basic equations are sometimes neglected based on research area of interest. Transient flow models of some selected problem was investigated (Kessal, 2000). The simulation natural gas flow in pipeline was investigated by many researchers where temperature effect is neglected with governed by conservation forms of mass and momentum. A new method was presented by (Zhou and Adewumi, 1996) on horizontal natural gas flow pipe, in which the lost accuracy due to neglected term are recovered as shown in presented results.

In slow and fast transient flow of high pressure of natural gas at nonisothermal condition overestimation was observed for steady state assumption on heat transfer was (Chaczykowski, 2010). Fully implicit finite difference method base on Newton-Raphson method in calculating transient flow behaviour of natural gas was investigated where greater reduction on computation time is achieved (Kiuchi, 1994)

Pipes sometime aged and got leak or failure due to corrosion or rupture A sensor PipeNet system was developed to detect leakage and failure so as to reduce the millions of dollar spends on monitoring water pipeline (Stoianov et al., 2007). Similar sensor can also be used in gas pipeline. Two monitoring methods are developed for location of leak pipe distance from transient flow simulation which demonstrate significant accuracy in detecting and locating of pipe leakage (Jang et al., 2010). The two methods are cross correlation monitoring and pressure differential monitoring methods.



The thermodynamic property of hydrogen is significantly different compared to that of natural gas. Robustness and mechanical resistance of natural gas was researched. Proper investigation is required since different thermodynamic properties are involved in the transient regime of hydrogen natural gas mixture (Elaoud and Hadj-Tai"eb, 2008).

The numerical investigation of high pressure hydrogen natural gas mixture was presented by (Elaoud and Hadj-Tai"eb, 2008) where pressure and velocity dependent variables are analysed. The thermal condition of hydrogen natural gas mixture was presented where hydrogen is injected into transient natural gas. By using the predictive Soave-Redlich-Kwong method (Uilhoorn, 2009).

There is a need for more research on transportation, production and storage capacity of hydrogen in order to meet with increasing the transformation of hydrogen becoming a major energy source of world economy. This can be achieved mostly in the transportation sector going by the existing sources. Although it will take decades before significant impact is made on the world economy (Wang, 2011).

Hydrogen and natural gas mixture (HCNG) of high pressure requires accurate prediction of fluid pressure and velocity variation. The transient flow of HCNG is as a result of rapid closure and opening of valves in meeting consumer demands. With the present of high capacity computer and programming languages such as MATLAB has been used in analysing transient behaviour of gas flow. PDEtoolbox can be used in prediction of HCNG transient flow parameter. How do we reduce computational cost as to computational scheme methods?

### **Numerical Technique**

Literature review as shown the importance of accuracy in flow problem. The numerical technique contributes significantly in finding solutions to various problems. For optimal operation of gas accuracy of pressure drop prediction is highly required. The efficiency and accuracy of natural transient flow using transient was investigated. (Behbahani-Nejad and Bagheri, 2010, Behbahani-Nejad and Shekari, 2010). Many mathematical models are continuously developed by researchers where different methods are used aimed at improvement of accuracy in flow parameters.

One dimensional model has been proven to be sufficient in the analysis of transient flow of natural gas flow. In the research conducted by (Thorley and Tiley, 1987) a literature review was excellently carried out on transient flow problem solution methods. Where characteristic method has shown an advantage on discontinuous flow cases, such as leakage or sudden cut, but relatively slow. The method with less accuracy is the explicit finite difference methods on transient flow problems, while Galerkin finite element is not commonly used in gas flow problems due to its computational storage demand. (Abbaspour et al., 2010)

The Reduce Order Modelling (ROM) technique has been demonstrating a high degree of accuracy in computation fluid problems. With computational efficiency and less cost, compared to other numerical methods. Usually achieved by transforming a large number of primitive variables into smaller amount at decoupled equations (Romanowski and Dowell, 1997). The ROM is constructed using Eigen analytical therefore few nodes are retained from the original nodes. The ROM is often used in aerodynamic problem but was introduced to gas flow problem and significant accuracy was presented. The analysis of aerodynamic problem, design of the wing fuselage system



and exhibited a low cost in computation of ROM (Jun et al., 2010). It also can be applied in analysis of subsonic flow.

From the concept of computation fluid dynamics equations that are mostly involve in fluids analysis are the Euler and the Navier-Stokes equations. The conservation forms of these equations are usually nonlinear hyperbolic partial differential equation which cannot be solve using the MATLAB command code PDENONLIN. (Kaist, 2012). MATLAB Simulink demonstrated efficiency on natural gas transient flow on pipeline network.

### Problem Formulation

The transportation of gas mixture is governed by conservation laws in pipeline, hence mass conservation equation and momentum will be involved while the non-isothermal conditions shall be ignored. Therefore, the governing equations on transportation of high pressured hydrogen natural gas mixture are as follows

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \underline{u} = 0 \quad (1a)$$

$$\frac{\partial(\rho \underline{u})}{\partial t} + (\underline{u} \cdot \nabla) \rho \underline{u} = \frac{\partial \sigma_{ij}}{\partial x_j} + F_j \quad (2a)$$

Since the isothermal condition is assumed with polytropic process on homogenous mixed condition that makes the fluid to be inviscid fluid hence one dimensional Euler equation will be sufficient in the analysis (Zhou and Adewumi, 1996, Osiadacz and Chaczykowski, 1998)

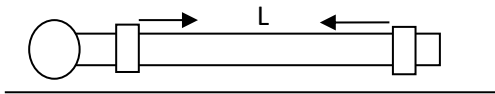


Figure1: Pipe geometry

Assuming an inviscid fluid of gas mixture, then the transient flow behaviour will be one dimensional conservation forms of Euler's continuity and momentum equations neglecting the body force.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (1b)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} = \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( f \frac{\partial u}{\partial x} + 2\mu \frac{\partial u}{\partial x} \right) + \rho f_x = 0 \quad (2b)$$

Using hypothesis of Stokes  $f = -\frac{2}{3}\mu$  (2.2b) becomes

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} = \frac{\partial p}{\partial x} - 2f \frac{\partial^2 u}{\partial x^2} + f_x g \quad (2c)$$

For  $p = \rho c^2$ , where  $c$  is the fluid celerity wave (2c) becomes



$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + c^2 \rho)}{\partial x} + \frac{f \rho u |u|}{2d} = 0 \quad (2d)$$

where  $\rho$  and  $u$  are fluid mixture density, velocity and  $f$  pipe friction factor respectively, (Behbahani-Nejad & Shekari, 2010)

For homogenous mixture of hydrogen natural, gas mixture density will be based on fluid mass ratio. We take into account hydrogen fluid mass ratio in this research to determining mixture density.

$$\varphi = m_h / (m_h + m_g) \quad (3a)$$

where  $m_g$ ,  $m_h$  are natural gas mass, hydrogen mass present and  $\varphi$  mass ratio (Elaoud et al., 2010, Elaoud and Hadj-Tai'eb, 2008).

Considering a polytropic process of gas flow then the density of each gas present will be

$$\rho_{h_0} = \rho_{h_p} \left( \frac{p}{p_0} \right)^{\frac{1}{nh}} \quad (3b)$$

$$\rho_{g_0} = \rho_{g_p} \left( \frac{p}{p_0} \right)^{\frac{1}{ng}} \quad (3c)$$

where  $\rho_{h_p}$ ,  $\rho_{g_p}$ ,  $\rho_{h_0}$ ,  $\rho_{g_0}$  are densities of hydrogen and natural gas at initial and permanent regime while  $p$ ,  $p_0$ ,  $nh$  and  $ng$  are transient regime pressure, permanent regime pressure, specific heat ratio of hydrogen and natural gas respectively.

The mixture density is then given by

$$\rho = \left[ \frac{\phi}{\rho_h} + \frac{1-\phi}{\rho_g} \right]^{-1} = \left[ \frac{\phi}{\rho_{h_0} \left( \frac{p}{p_0} \right)^{\frac{1}{nh}}} + \frac{(1-\phi)}{\rho_{g_0} \left( \frac{p}{p_0} \right)^{\frac{1}{ng}}} \right]^{-1} \quad (4)$$

(Elaoud and Hadj-Tai'eb, 2008)

The celerity pressure of compressible gas fluid is define as

$$c' = \left( \frac{d\rho}{dp} \right)^{\frac{1}{2}} \quad (5)$$

Differentiating 4 and substituting into 5 we have

$$c' = \left[ \frac{\phi}{\rho_{h_0} \left( \frac{p}{p_0} \right)^{\frac{1}{nh}}} + \frac{(1-\phi)}{\rho_{g_0} \left( \frac{p}{p_0} \right)^{\frac{1}{ng}}} \right] \times \left[ \frac{1}{p} \left[ \frac{\phi}{nh \rho_{h_0} \left( \frac{p}{p_0} \right)^{\frac{1}{nh}}} + \frac{(1-\phi)}{ng \rho_{g_0} \left( \frac{p}{p_0} \right)^{\frac{1}{ng}}} \right] \right]^{-\frac{1}{2}} \quad (6)$$

(Elaoud and Hadj-Tai'eb, 2008)

Every flow is initially at steady state condition therefore the transient flow of HCNG is assumed



Initial conditions:

$$\frac{\partial \rho(x, 0)}{\partial x} = 0 \quad (7a)$$

$$\frac{\partial \rho v(x, 0)}{\partial x} = -c'^2 \frac{\partial \rho}{\partial x} - f \frac{\rho v^2}{2D} \quad (7b)$$

Boundary conditions are known to be depending on valves operational time and locations couple with compressor supply and pressure regulator. In these research valves are place in upstream and downstream of pipe.

For a closure downstream valve and while upstream valve remain open boundary conditions are

$$P(0, t) = P_0 (\text{known function}) \quad (8a)$$

$$\frac{\partial(\rho u)}{\partial x} = (\rho u)_0 (\text{known function}) \quad (8b)$$

$$\frac{\partial p(L, t)}{\partial x} = 0 \quad (8c)$$

$$\rho(L, t) = \rho_L(t) \quad (8d)$$

### Finite Element Form

Before partial differential equation toolbox can be used, both the governing equation and boundary conditions have to be rewritten in finite element format.

Rewriting the equations in the form

$$U_t - \text{div}(c \otimes \text{grad}(U)) + aU = F \quad (9)$$

Where

$$U = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}; f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}; a = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}; c = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}; d = \begin{pmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{pmatrix}$$

Writing equations 1b and 2d in matrix form

$$\frac{\partial Q}{\partial t} + \frac{\partial E(Q)}{\partial x} - H(Q) = 0 \quad (10)$$

$$\text{where } Q = \begin{pmatrix} \rho \\ \rho u \end{pmatrix} = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \quad (11a)$$

$$E(Q) = \begin{pmatrix} q_2 \\ \frac{q_2^2}{q_1} + c'^2 q_1 \end{pmatrix} \quad (11b)$$



$$H(Q) = \begin{pmatrix} 0 \\ -\frac{q_2 f |q_2|}{2q_1 D} \end{pmatrix} \quad (11c)$$

$$d_{11} \frac{\partial q_1}{\partial t} + d_{12} \frac{\partial q_2}{\partial t} - c_{11} \frac{\partial q_1}{\partial x} - c_{12} \frac{\partial q_2}{\partial x} + a_{11} q_1 + a_{12} q_2 = f_1 \quad (12a)$$

$$d_{21} \frac{\partial q_1}{\partial t} + d_{22} \frac{\partial q_2}{\partial t} - c_{21} \frac{\partial q_1}{\partial x} - c_{22} \frac{\partial q_2}{\partial x} + a_{21} q_1 + a_{22} q_2 = f_2 \quad (12b)$$

$$\begin{bmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial q_1}{\partial t} \\ \frac{\partial q_2}{\partial t} \end{bmatrix} - \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial q_1}{\partial x} \\ \frac{\partial q_2}{\partial x} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \quad (13)$$

becomes

$$dQ_t - \nabla \cdot (c \otimes \nabla) + aQ = F \quad (14)$$

$$\frac{\partial q_1}{\partial t} + 0 \frac{\partial q_2}{\partial t} - \frac{\partial q_1}{\partial x} - (-1) \frac{\partial q_2}{\partial x} + 0q_1 + 0q_2 = 0 \quad (15a)$$

$$\frac{\partial q_1}{\partial t} + \frac{\partial q_2}{\partial t} - (-c'^2) \frac{\partial q_1}{\partial x} - \left(2 \frac{q_2}{q_1}\right) \frac{\partial q_2}{\partial x} + 0q_1 + \left(-\frac{f|q_2|}{2q_1}\right) q_2 = 0 \quad (15b)$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial q_1}{\partial t} \\ \frac{\partial q_2}{\partial t} \end{bmatrix} - \begin{bmatrix} 0 & -1 \\ -c'^2 & -2 \frac{q_2}{q_1} \end{bmatrix} \begin{bmatrix} \frac{\partial q_1}{\partial x} \\ \frac{\partial q_2}{\partial x} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \frac{f|q_2|}{2q_1} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (16)$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} Q_t - \nabla \cdot \left( \begin{bmatrix} 0 & -1 \\ -c'^2 & -2 \frac{q_2}{q_1} \end{bmatrix} \otimes \nabla \right) + \begin{bmatrix} 0 & 0 \\ 0 & \frac{f|q_2|}{2q_1} \end{bmatrix} Q = \begin{bmatrix} 0 \\ 0 \end{bmatrix} F \quad (17)$$

(17) is nonlinear and PDEtool does NOT support nonlinear hyperbolic and parabolic PDE's (Kaist, 2012, Yang et al., 2005)

Therefore, a process of linearization will be employed, such that (17) becomes

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} Q_t - \nabla \cdot \left( \begin{bmatrix} 0 & -1 \\ -c'^2 & -2 \frac{q'_2}{q'_1} \end{bmatrix} \otimes \nabla \right) + \begin{bmatrix} 0 & 0 \\ 0 & \frac{f|q'_2|}{2q'_1} \end{bmatrix} Q = \begin{bmatrix} 0 \\ 0 \end{bmatrix} F \quad (18)$$

where  $q'_1$  and  $q'_2$  are steady state solution (1) and (2d)

Boundary Condition will be written in Finite Element Form

Therefore

$$c_{11} = 0, \quad c_{12} = u_2, \quad c_{21} = -C^2 u_1, \quad c_{22} = uu_2$$

$$a_{11} = 0, \quad a_{12} = 0, \quad a_{21} = 0, \quad a_{22} = u_x - \frac{uf}{2d}$$



$$f_1 = 0, f_2 = 0, d_{11} = 1, d_{12} = 0, d_{21} = 0, d_{22} = 1$$

Used GUI to obtain the boundary matrix and the geometry composition of the define problem on the given domain, of the pipe dimension of  $d=0.61$  with length  $91.44\text{m}$ . This is used in the command syntax that solves nonlinear partial differential equations.

The concept of Newton iteration with Armijo-Goldstein line algorithm is used by the command.

Using GUI to obtain the boundary matrix and the mesh parameters hence exported to MATLAB M-file command. The nonlinear parts are handle using pdeintpr command.

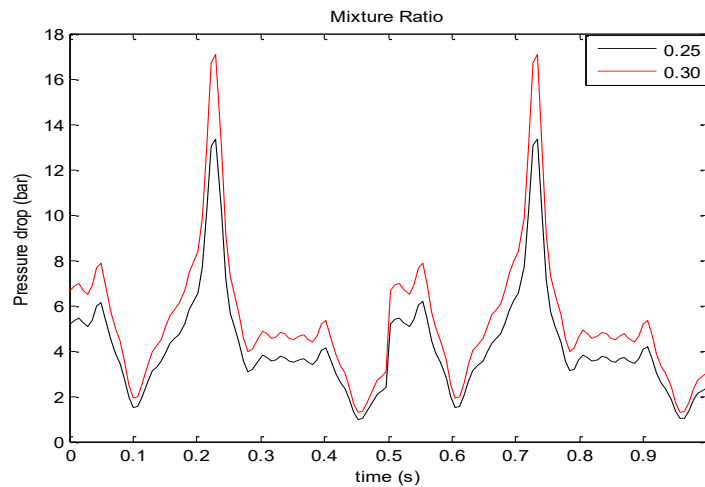


Figure 1: Effect of Hydrogen present on gas mixture pressure drop.

The pressure drop is constantly effected by hydrogen present throughout the simulation process, as it can be observed from figure 1 only at time 0.54 second of the entire process. The highest pressure drop is observe at 0.25 and 0.75 seconds that is the first and last quarter of the process. The figure is observed to be a sinusoidal

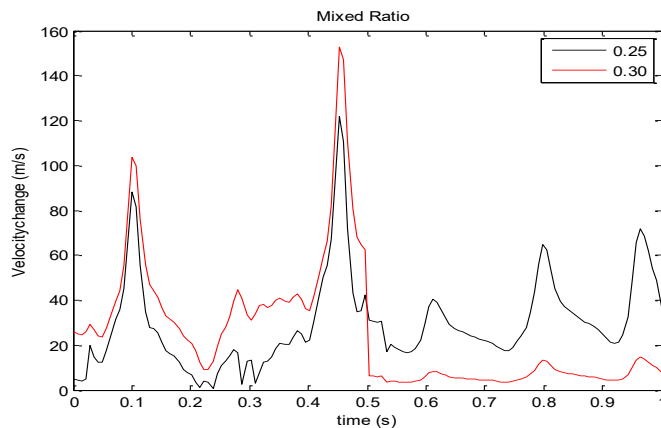


Figure 2: Effect of hydrogen present on gas mixture Velocity change





The velocity change at beginning of simulation is higher for increase in hydrogen present this is as a result of high burning ration and low density of hydrogen. It stabilized after sometimes during the simulation process.

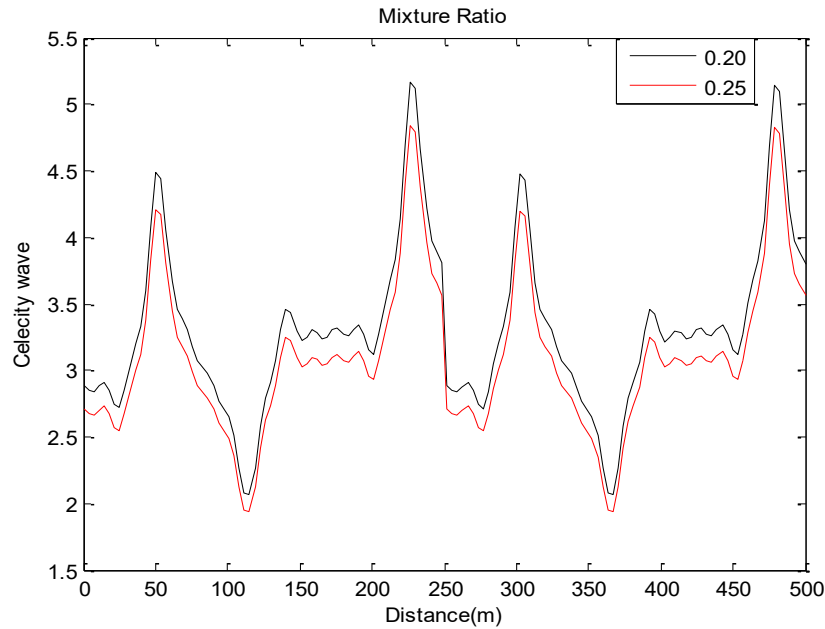


Figure 3: Effect of hydrogen present on gas mixture Celerity wave

The effect hydrogen on celerity wave is constant throughout the simulation process. At mid-point of the pipeline the celerity is equal for different in hydrogen percentage present during the flow.

#### Problem 2

##### Inclination of pipeline

In this problem the momentum equation varies from equation (2) to take carry of the incline angle and becomes

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + c^2 \rho)}{\partial x} + \frac{f \rho u |u|}{2d} - \rho g \sin \theta = 0 \quad (2e)$$

The process follows to obtain the result is as above equations 17 which becomes

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} Q_t - \nabla \cdot \left( \begin{bmatrix} 0 & -1 \\ -c^2 & -2 \frac{q_2}{q_1} \end{bmatrix} \otimes \nabla \right) + \begin{bmatrix} 0 & 0 \\ 0 & \frac{f|q_2|}{2q_1} - \rho g \sin \theta \end{bmatrix} Q = \begin{bmatrix} 0 \\ 0 \end{bmatrix} F \quad (19)$$

Linearizing (19) as in (17) we have

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} Q_t - \nabla \cdot \left( \begin{bmatrix} 0 & -1 \\ -c'^2 & -2 \frac{q'_2}{q'_1} \end{bmatrix} \otimes \nabla \right) + \begin{bmatrix} 0 & 0 \\ 0 & \frac{f|q'_2|}{2q'_1} - \rho g \sin \theta \end{bmatrix} Q = \begin{bmatrix} 0 \\ 0 \end{bmatrix} F \quad (20)$$

with  $q'_1$  and  $q'_2$  are steady state solution obtain from (1) and (2d)

## Results and Discussions

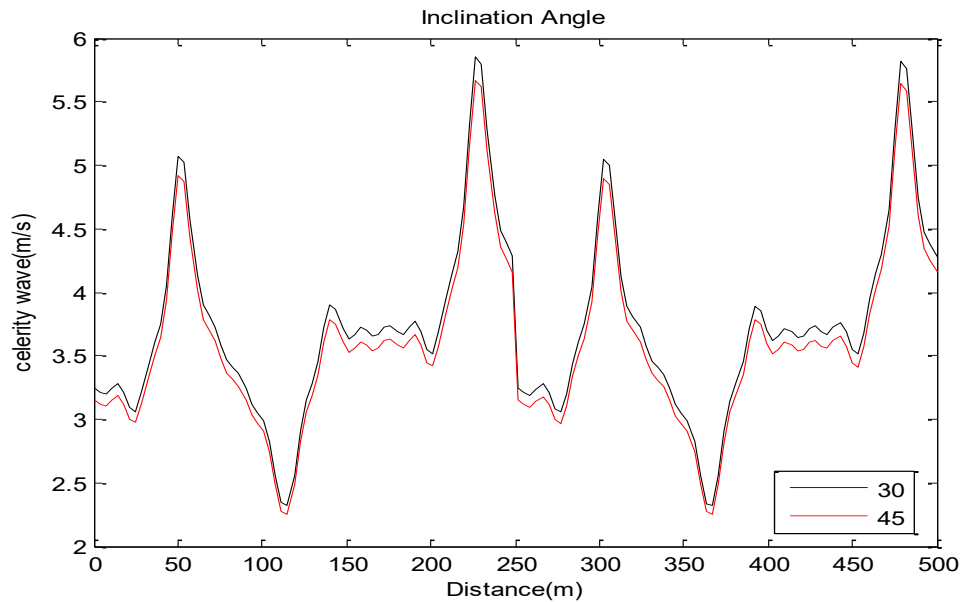


Figure 4: Effect of inclination angle on gas mixture Celerity wave

The effect of inclined angle can be observed in the celerity wave of the pipeline system. From figure 4 the inclined angle is varies by a different of just  $5^\circ$  but the clearly show variation in the velocity wave.

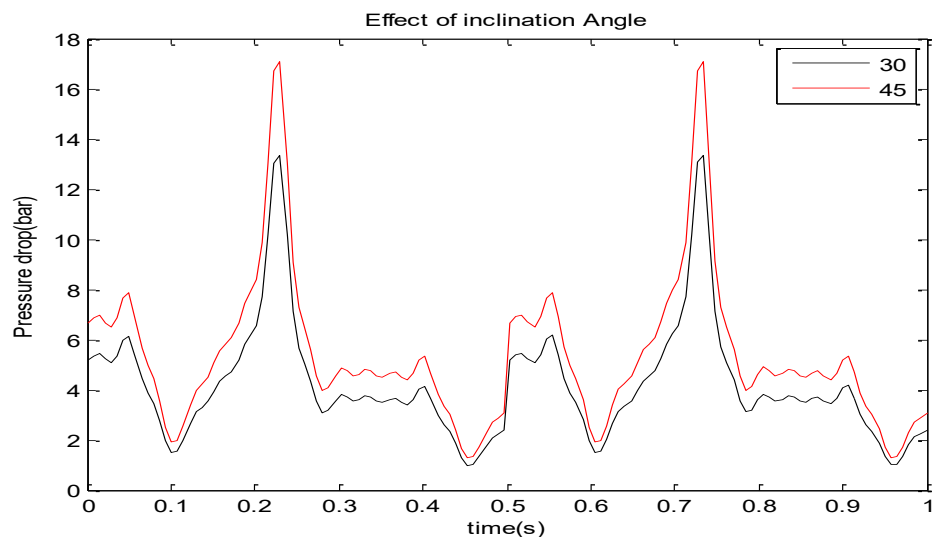


Figure 5: Effect of inclination angle on gas mixture pressure drop

There is similarity of the pressure drop effect as to velocity wave as presented in figure 4 when the same inclination angles are varies.

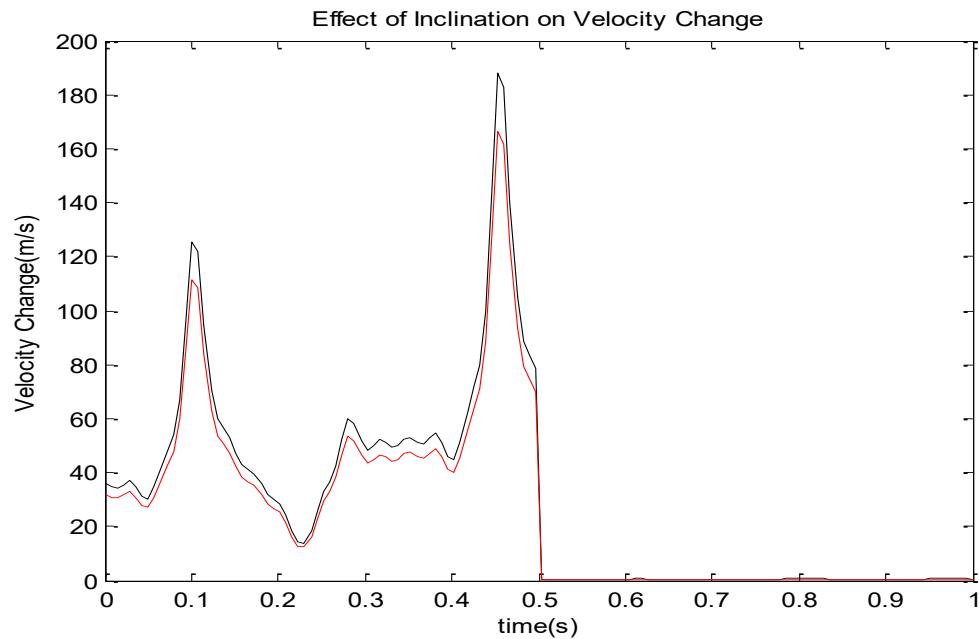


Figure 6: Effect of inclination angle on gas mixture velocity change  
From figure 6 the inclined affect the velocity change in each nodal point and converge at mid-point of the pipe length.

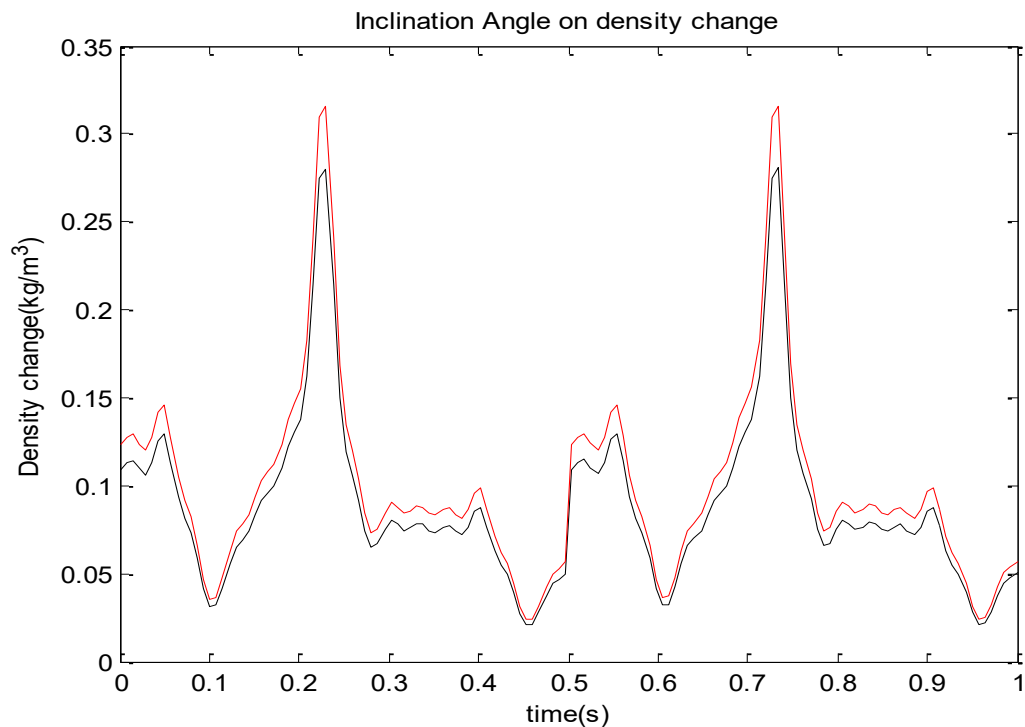


Figure 7: Effect of inclination angle on gas mixture density change



From figure 7 the density change during flow at nodal point has no significant change on graph due to different in inclined angles

### Conclusion and Recommendation

From the simulated results PDEtool show a significant accuracy is the simulation of transient flow of hydrogen natural gas problems. The tool show to improve on accurate prediction of flow parameters. It is therefore recommended for simulation of flow related problem which can also be extended to system of three PDE that is when energy equation is involved to makes the problem a real life problem.

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