TRANSIENT FLOW IN PIPELINES OF HIGH-PRESSURE HYDROGEN AND NATURAL GAS MIXTURE

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ABSTRACT
The purpose of this study is the numerical modeling of high-pressure transient flow in rigid pipelines of hydrogen and natural gas mixture. The governing equations for such flows are two coupled, non linear, hyperbolic, partial differential equations. The fluid pressure and velocity are considered as two principal dependent variables. The fluid is a homogeneous hydrogen-natural gas mixture for which the density is defined by an expression averaging the two gas densities where a polytropic process is admitted. The problem has been solved by the finite difference method of Lax-Wendroff and the method of characteristics. The occurrence of pressure oscillations in gas mixture pipelines was studied as a result of the compression wave created by the rapid closure of downstream shut-off valve.

1.0 INTRODUCTION
Today, hydrogen is considered the most abundant and clean gas. Many researches are concentrated in its production, storage and transportation. As a manner of economic way, many petroleum companies utilize the existing pipelines, normally used to transport natural gas, in transporting hydrogen mixed with natural gas. In this paper, we study the transient flow of the gas mixture for different values of hydrogen mass fraction. The transient regime is created by the rapid closure of a downstream shut-off valve. The numerical simulation was performed by solving the conservation equations using two methods: the finite difference method of Lax-Wendroff and the characteristics irregular grid method. The pipe is considered rigid.

2.0 HYPOTHESES
The transient flow is supposed one-dimensional and concerns a homogeneous fluid mixture of hydrogen and natural gas. The calculation of the pressure loss is done by analogy with the permanent flows. The hydrogen-fluid mass ratio (or the quality) is noted \( \theta = \frac{M_h}{M_g + M_h} \) where \( M_h \) and \( M_g \) represent the masses of hydrogen and natural gas respectively. The density of hydrogen and natural gas evolve according to the following polytropic laws:

\[
\rho_h = \rho_{ho} \left( \frac{p}{p_o} \right)^{1/n}, \quad (1)
\]

\[
\rho_g = \rho_{go} \left( \frac{p}{p_o} \right)^{1/n'}, \quad (2)
\]

where \( \rho_{ho} \) – density of hydrogen at the initial conditions, kg/m\(^3\); \( \rho_{go} \) – density of natural gas at the initial conditions, kg/m\(^3\); \( p_o \) – permanent regime pressure, N/m\(^2\).

The pipe is supposed to be rigid, that means that the section \( A \) of the pipe is constant:

\[
A = A_o = \frac{\pi D^2}{4} = cte \quad (3)
\]

where \( D \) – diameter of the pipe, m.
3.0 MATHEMATICAL FORMULATION

3.1 Momentum equations

By application of the mass conservation and momentum laws to an element of fluid between two sections of abscissa \( x \) and \( x+dx \) of the pipe, we get the following equations of continuity and motion \([1]\):

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho V}{\partial x} = 0
\] (4)

\[
\frac{\partial \rho V}{\partial t} + \frac{\partial (\rho V^2 + p)}{\partial x} + \frac{\lambda \rho V |V|}{2D} = 0
\] (5)

where \( \lambda \) – coefficient of friction; \( V \) – velocity of the mixture, m/s.

Equations (4) and (5) form a system of two non-linear partial differential equations of hyperbolic type in which the pressure \( p \) and the velocity \( V \) are considered the main variables of the flow. To solve numerically these equations, we must express the density of the mixture \( \rho \) according to the fluid pressure.

3.2 Expression of the mixture density

The expression of the average density of the mixture is defined according to the hydrogen mass ratio \( \theta \) \([2]\).

\[
\rho = \left[ \frac{\theta}{\rho_h} + \frac{1-\theta}{\rho_g} \right]^{-1}
\] (6)

3.3 Expression of the celerity of pressure waves

For a compressible fluid, the celerity of the pressure waves can be defined by the expression:

\[
C^2 = \left( \frac{\partial \rho}{\partial p} \right)^{-1}
\] (7)

Taking into account the relations (1), (2), (6), and (7), we obtain:

\[
C = \left[ \frac{\theta}{\rho_{ho}} \left( \frac{p}{p_o} \right)^{1/n'} + \frac{1-\theta}{\rho_{go}} \left( \frac{p}{p_o} \right)^{1/n} \right]^{1/2}
\] (8)

4.0 METHOD OF CHARACTERISTICS

The method of characteristics is often used to transform the governing partial differential equations (4) and (5) into a system of ordinary differential equations that are valid along two sets of characteristic lines (figure 1). The ordinary differential equations obtained by this method are \([3, 4]\):

\[
\begin{cases}
C + \frac{1}{\rho C} dp = -J dt \\
dx = (V + C) dt
\end{cases}
\] (9)
\[
\begin{align*}
C^- & \left\{ \frac{dV}{\rho C} - \frac{1}{dp} = -Jdt, \\
& \quad dx = (V - C)dt \right. \\
\end{align*}
\]  

(10)

where \( J = \lambda V|V|/2D \) – represents the pressure loss by unit of pipe length, m.s\(^{-2}\).

These equations can also be written under the following form:

\[
\begin{align*}
dV \pm \frac{1}{\rho C} dp - J dt = 0 \quad \text{and} \quad dx = (V \pm C) dt \end{align*}
\]  

(11)

The + is for the waves coming from the upstream while the - is for the waves coming from the downstream.

Equations (11) determine the evolution of the pressure and the velocity according to the time and the space. They are much appropriated to be solved numerically on a microcomputer. The obtained solution constitutes a solution to the original system of the equations (4) and (5).

The transient flow is generated by a discontinuity of the steady state flow due to a rapid valve closure. This discontinuity propagates itself and the displacement is presented in the plan \((x, t)\) by the characteristic lines.

The unknown values of \((V, p, x, t)\), at any point \(P\), as shown in figure 1, can be determined by knowing their values at the points \(R\) and \(S\) lying on the two characteristics passing through \(P\) and by integrating the two simultaneous equations (9) and (10). These equations can be written for the two signs, which results in four finite difference equations:

\[
\begin{align*}
(V_p - V_R) + \int_R^P \frac{dp}{\rho C} + \int_P^R J dt & = 0 \\
(x_p - x_R) & = \int_R^P (V + C) dt \end{align*}
\]  

(12) (13)

\[
\begin{align*}
(V_p - V_S) + \int_S^P \frac{dp}{\rho C} + \int_P^S J dt & = 0 \\
(x_p - x_S) & = \int_S^P (V - C) dt \end{align*}
\]  

(14) (15)

As the characteristics are curved on the \((x, t)\) plane due to the non-linearity of equations (4) and (5), the integration is achieved by means of an iterative trapezoidal rule.

Consequently, we obtain the unknown values \(t_P, x_P, V_P\) and \(p_P\) at the point \(P\):

\[
t_P^k = \frac{x_S - x_R + F_R t_R - G_S t_S}{F_R - G_S} \\
(16)
\]

\[
x_P^k = x_R + F_R \left( t_P^k - t_R \right) \\
(17)
\]
\[
p^k_p = \frac{M_R p_R + M_S p_S + V_R - V_S + H_R \left( \frac{k}{s} - t_R \right) - H_S \left( \frac{k}{s} - t_S \right)}{M_R + M_S}
\]  
(18)

\[
V^k_p = V_R + M_R \left( p_R - p^k_p \right) + H_R \left( \frac{k}{s} - t_R \right)
\]  
(19)

where: \( F_R = (V + C)_R \), \( G_S = (V - C)_S \), \( M_{R,S} = \left( \frac{1}{\rho} C \right)_{R,S} \), \( H_{R,S} = -J_{R,S} \) for \( k = 1 \)

and \( F_R = \frac{1}{2} \left[ (V + C)_R^{k-1} + (V + C)_R \right] \), \( G_S = \frac{1}{2} \left[ (V - C)_S^{k-1} + (V - C)_S \right] \)

\[
M_{R,S} = \frac{1}{2} \left[ \left( \frac{1}{\rho} C \right)_R^{k-1} + \left( \frac{1}{\rho} C \right)_{R,S} \right] \), \( H_{R,S} = \frac{1}{2} \left[ (-J)_R^{k-1} + (-J)_{R,S} \right] \) for \( k = 2 \ldots m \)

In this study, the iteration number is limited to \( m = 20 \).

The determination of the solution in the two extreme sections imposes the introduction of the appropriate boundary conditions.

**5.0 FINITE DIFFERENCE METHOD (LAX-WENROFF SCHEME)**

The finite difference method is applied only for equations which can be written in the so-called conservative form:

\[
\frac{\partial U}{\partial t} + \frac{\partial W(U)}{\partial t} = S(U),
\]  
(20)

where \( U \) is the vector of conservative variables, \( W \) is the flux vector, and \( S \) the source term. The equations (4) and (5) of continuity and motion can be written under the conservative form (20) where:

\[
U = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = \begin{pmatrix} \rho \\ \rho V \end{pmatrix}
\]  
(21)

\[
W = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix} = \begin{pmatrix} \rho \\ \frac{(\rho V)^2}{\rho} + p \end{pmatrix}
\]  
(22)
Once written under the conservative form, equations (4) and (5) can be solved by two-step finite difference \( S^\alpha_\beta \) scheme [5]. Indeed, with the notations of figure 2, we can write: \( U_i^k = U(i\Delta x,k\Delta t) \) and \( W_i^k = W(U_i^k) \). Moreover, the unknown vector \( U(x,t) \) can be approximated with the first two terms of its Taylor expansion about \( t \), as follows:

\[
U(x,t+\Delta t) = U(x,t) + \Delta t \frac{\partial U}{\partial t}
\]

(24)

Then, by introducing the physical laws of the transient flow, that is:

\[
\frac{\partial U}{\partial t} = \frac{\partial W(U)}{\partial t} + S
\]

(25)

We obtain the finite difference form:

\[
U(x,t+\Delta t) = U(x,t) - \Delta t \frac{\partial W}{\partial x} + \Delta t S
\]

(26)

The Lax-Wendroff scheme is a particular case of the finite difference method, it corresponds to a couple \((\alpha,\beta) = (1/2,1/2)\) and the solution is as follows:

\[
\tilde{U}_{i+1}^{k+1/2} = \frac{1}{2} \left( U_i^k + U_{i+1}^k \right) - \frac{\sigma}{2} \left( W_{i+1}^k - W_i^k \right) + \frac{1}{2} \Delta t S_i^k
\]

(27)

\[
U_i^{k+1} = U_i^k - \sigma \left( \tilde{W}_{i+1}^k - \tilde{W}_{i-1}^k \right) + \Delta t S_i^k
\]

(28)

where \( \sigma = \Delta t / \Delta x \) – the grid mesh ratio, \( s/m \).

The scheme is a three point explicit method of second-order accuracy. It can be shown that the requirement condition for stability is given by Courant-Friedrichs-Lewy condition [6]:

\[
\frac{\Delta t}{\Delta x} \leq \frac{1}{|V| + C)_{max}}
\]

(25)

Figure 2. Finite difference scheme
6.0 APPLICATIONS AND RESULTS

6.1 Description of the system and position of the problem

To illustrate the dynamic behavior of high-pressure hydrogen-natural gas mixture in pipelines, we consider an installation (fig 3) composed with a compressor pumping the mixture through an iron pipe of 0.4 m in diameter and 500 m long. In the event of a sudden emergency, we place at the downstream end a rapid closure valve (RCV). In this case, the pressure in the supply line may reach excessive values and may destroy the compressor and the pipeline. To avoid this, we place at the immediate discharge side of the compressor, an automatic closure valve (ACV). As initial condition, we assume a mass flow \( m_0 = 10 \text{ Kg/s} \) (398714.400 m\(^3\)/(n)/s), a static temperature \( T = 15°C \) and an absolute pressure \( p = 20 \text{ bar} \). Properties of hydrogen and natural gas used in the calculations are presented in Table 1 and Table 2 respectively [7].

Table 1. Hydrogen properties in working conditions \( p = 20 \text{ bar} \) and \( T = 15°C \)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Designation</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_p )</td>
<td>Specific heat at constant pressure</td>
<td>14600</td>
<td>J/(Kg °K)</td>
</tr>
<tr>
<td>( C_v )</td>
<td>Specific heat at constant volume</td>
<td>10440</td>
<td>J/(Kg °K)</td>
</tr>
<tr>
<td>( R )</td>
<td>gas constant</td>
<td>4160</td>
<td>J/(Kg °K)</td>
</tr>
</tbody>
</table>

Table 2. Natural gas properties in working conditions \( p = 20 \text{ bar} \) and \( T = 15°C \)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Designation</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_p )</td>
<td>Specific heat at constant pressure</td>
<td>1056.8</td>
<td>J/(Kg °K)</td>
</tr>
<tr>
<td>( C_v )</td>
<td>Specific heat at constant volume</td>
<td>1497.5</td>
<td>J/(Kg °K)</td>
</tr>
<tr>
<td>( R )</td>
<td>gas constant</td>
<td>440.7</td>
<td>J/(Kg °K)</td>
</tr>
</tbody>
</table>

Two parameters were used to characterize the dynamic response of the valves: the reaction time (time taken to start the valve actuation after sensing a pressure perturbation) and the actuation time (time interval between the initial and the final positions of the valve). For the RCV we considered the actuation time only. The Table 3 summarizes these closure times.

Table 3. Reaction and actuation time of valves

<table>
<thead>
<tr>
<th>Case</th>
<th>ACV reaction</th>
<th>ACV actuation</th>
<th>RCV actuation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2 sec</td>
<td>5 sec</td>
<td>0.25 sec</td>
</tr>
<tr>
<td>2</td>
<td>0.2 sec</td>
<td>0.5 sec</td>
<td>0.2 sec</td>
</tr>
</tbody>
</table>

Figure 3. Gas installation
6.2 Results and discussion

Referring to the Table 3, we consider a linear variation of the mass-flow during the valve transient. Figures 4 and 5 show plots of the numerically obtained results for the variation of the mass-flow for cases 1 and 2, as functions of time, for two sections at the exit side of the automatic closure valve (ACV) and immediately upstream end of the emergency rapid closure valve (RCV). The figure 4 shows the influence of the hydrogen mass ratio $\theta$ in the closing time of the (ACV), this, is due to the variation of the pressure wave celerity which is proportional to the hydrogen mass ratio $\theta$.

Figures 6, 7 and 8, show plots of the pressure distribution for the cases 1 and 2, as a function of time and for different values of the hydrogen mass ratio $\theta$, at the (ACV) side, the middle of the pipe and the (RCV) side respectively. The numerical results clearly show the interaction of the pressure wave, generated by the rapid closure of the (RCV), with the closure time of the (ACV). Also we can clearly see the influence of the hydrogen mass ratio $\theta$ on the maximum value of pressure.

On the figure 6, for $\theta=1$, and for the case 1, the value of the maximum pressure predicted at the (ACV) is 33.2 bar, which is reached after 7.53 seconds after the valve closure. In this example, the increase in mass in the system, due to delay of the (ACV) closure, generates a pressure increase much higher than that due to the rapid closure of the (RCV). This over pressure, by mass accumulation, may
be reduced by reducing the closure time of the upstream valve which is represented by the case 2. Also, the plots represented on the figure 6, show the influence of the value of \( \theta \). We can see that, for the case 1, the maximum pressure passes from 22 bar for \( \theta = 0 \) to 33.2 bar for \( \theta = 1 \).

In the other sections of the pipe, we can note the same influence of the time closure of valves and the different values of \( \theta \) on the pressure evolution.

The figure 7 shows the influence of the superposition of the two waves reflected from the upstream side and the downstream side of the pipe. These waves came upon the middle of the pipe causing a neutralization effect which reduces the pressure fluctuations.

The plots of the figures 6, 7 and 8 also show the perfect concordance of the numerical results obtained by the method of characteristics (M.O.C) and the finite difference method (F.D).

Figures 9, 10 and 11 show the evolution of the characteristic lines grid for different values of the hydrogen mass ratio \( \theta \). It can be seen that as much as \( \theta \) close to 1, as high as the celerity of waves is.

Figure 6. Pressure as a function of time for cases 1 and 2 at the (ACV) side for different values of \( \theta \)
Figure 7. Pressure as a function of time for cases 1 and 2 at the middle of the pipe for different values of $\theta$.

Figure 8. Pressure as a function of time for cases 1 and 2 at the (RCV) side for different values of $\theta$. 

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Figure 9. Evolution of characteristic lines in cases 1 and 2 for $\theta = 0$

Figure 10. Evolution of characteristic lines in cases 1 and 2 for $\theta = 0.6$
6.0 CONCLUSION

In this study, the numerical solution of the transient flow in rigid pipelines of natural gas and hydrogen mixture has been presented. This problem is governed by coupled two linear partial differential equations of hyperbolic type. The numerical methods employed are the method of characteristics and the finite difference method of Lax-Wendroff.

The boundary conditions were imposed by introducing a linear closure law for the upstream and the downstream valve.

The occurrence of pressure oscillations in the different sections of the pipe was analysed as a result of the compression wave originated by the rapid closure of downstream valve (RCV). In this case, the pressure may reach excessive values due to the mass accumulation effect caused by the delay of the upstream valve closure. We have also analysed the effect of the different values of hydrogen mass ratio $\theta$ on the dynamic behaviour of the pressure.

The plots presented show the perfect concordance of the numerical results obtained by the method of characteristics (M.O.C) and the finite difference method (F.D).

REFERENCES

