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ORIGINAL PAPER

Computational fluid dynamic modeling of methane-hydrogen mixture transportation in pipelines: estimating energy costs

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Abstract
Replacing fossil fuels and natural gas with alternative fuels like hydrogen is an important step toward the goal of reaching a carbon neutral economy. As an important intermediate step toward utilizing pure hydrogen, blending hydrogen in an existing natural gas network is a potential choice for reducing carbon emissions. A computational fluid dynamic model is developed to quantify frictional losses and energy efficiency of transport of methane-hydrogen blends across straight pipe sections. It is observed that, in general, an increase in the energy costs is expected when hydrogen, with its lower density, is transported along with methane (which has higher density) in various blend ratios. However, the amount of increase in energy costs depends on the volume fraction of hydrogen and the nature of the flow conditions. The lowest energy costs are projected for transporting pure hydrogen under the conditions where the inlet velocity flow rates are similar to that used for transporting pure methane while the highest energy costs are expected when hydrogen is transported at the same mass flow rate as methane.

Introduction

Replacing fossil fuels (such as natural gas) with non-carbon fuels (such as hydrogen) is an important step toward reaching the ultimate goal of carbon neutrality. It has been recognized that incremental blending of hydrogen with natural gas is one way of progressively reducing carbon emissions while providing a seamless transition with minimal disruptions in power and heating source distribution to the public. Consequently, several projects such as HyDeploy, GRHYD, THyGA, and Hyblend have focused on assessing the impacts and implications of hydrogen blending in the existing natural gas networks [1–6] that include storage and transportation and end-use applications. These projects have considered a combination of laboratory-scale studies and pilot-scale models.

Preliminary studies in hydrogen blending have demonstrated that end-use appliances such as modified engines, oven burners, boilers, stoves, and fuel cells can be designed to have good compatibility with hydrogen blended fuels where the blend volume fraction of hydrogen is typically around 20% or less. However, in considering higher blend concentrations of hydrogen in the natural gas—hydrogen mixtures, the advantages of hydrogen as a non-carbon energy carrier need to be balanced with safety concerns of blended gas during transport, such as overpressure and leakage in pipelines, hydrogen embrittlement issues and energy costs for transportation.

In general, experimental studies and modeling approaches are needed to fully understand the impact of higher hydrogen concentrations in the natural gas—hydrogen blends on the gas infrastructure. In particular, with the advances made by researchers and software developers in developing several turbulence models and multiphase models, computational fluid dynamics (CFD) modeling has the potential to provide insights on several aspects of the complex flow behavior of natural gas—hydrogen mixtures.

For example, Cadorin et al. [7] analyzed the flow behavior of natural gas—hydrogen mixtures with 10% hydrogen using CFD modeling. These researchers selected the

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standard $k-\varepsilon$ model for capturing the expected turbulence in the high Reynolds number flow regime. Their study also investigated three equations of state (EOS) of gases that included gases with constant properties, ideal gases, and Redlich–Kwong gases. It was demonstrated that the three equations of state of gases provided reasonably good results with the Redlich–Kwong EOS providing the best predictions among the three. Using the CFD results, they also assessed the energy transfer efficiency of natural gas and methane-hydrogen mixtures. In the study, a new metric was introduced—the energy specific toll (EST)—which represents the energy required to transport gases in a unit length of pipeline to offset the energy loss from frictional effects. They found that methane-hydrogen mixture (90% methane and 10% hydrogen) in high Reynolds number flow self-consumes almost two times more energy than natural gas.

While the work of Cadorin et al. provided interesting insights into the flow behavior of natural gas—hydrogen blends, their study was limited to one concentration of hydrogen and one particular geometry of pipe and limited flow boundary conditions. So, there is considerable interest in understanding the flow behavior of blends of various hydrogen concentrations in pipes of different sizes and with different operating boundary conditions.

Hence, the objectives of the present study were to: (i) develop and validate a three-dimensional CFD model for capturing the flow behavior of hydrogen-methane blends; (ii) systematically assess the effects of hydrogen concentration and flow boundary conditions on the blended gas flow characteristics such as pressure drops; and (iii) obtain insights on the energy efficiency of transportation of methane-hydrogen gas blends in straight horizontal pipe sections.

Numerical modeling

Governing equations

ANSYS FLUENT is the modeling software utilized in this study to simulate the methane-hydrogen mixture transportation in a pipeline section. The conservation of mass and momentum equations used in all CFD software are derivations of the Navier–Stokes equations. The conservation of mass or continuity equation of FLUENT (ANSYS FLUENT Theory Guide) is based on Eq. 1.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{v}\right) = S_m \tag{1}$$

In Eq. 1, the term ρ represents density, while v is the velocity vector. S_{m} is the source term, representing additional mass to the continuous phase, for example from phase transformation, or other sources defined by users.

A volume of fraction (VOF) model is used to describe the behavior of the methane-hydrogen mixture in the system. The advantage of the VOF model is that it only requires one set of momentum equations with tracking of volumetric fraction of each fluid in the flow domain to model a system of multiple immiscible fluids. In a VOF model, where multiple phases coexist in the system, the qth phase continuity equation can be expressed as given in Eq. 2.

$$\frac{1}{\rho_1}\left[\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla \cdot \left(\alpha_q \rho_q \vec{v}_q\right) = S_{\alpha_q} + \sum_{p=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right] \tag{2}$$

The term α_q represents the volume fraction of the qth phase. The mass transfer from phase q to phase p is expressed in the term $\dot{m}_{qp}$. The source term, S, can be defined for each phase. The conservation of momentum equation is listed below in Eq. 3.

$$\frac{\partial}{\partial t}\left(\rho \vec{v}\right) + \nabla \cdot \left(\rho \vec{v}\vec{v}\right) = -\nabla \mathrm{p} + \nabla \cdot \left(\overline{\overline{\tau}}\right) + \rho \vec{g} + \vec{F} \tag{3}$$

The term p represents the static pressure. Gravitational forces and external forces are captured by $\rho \vec{g}$ and $\vec{F}$. $\overline{\overline{\tau}}$ is the stress tensor explained in Eq. 4.

$$\overline{\overline{\tau}} = \mu\left[\left(\nabla \vec{v} + \nabla \vec{v}^T\right) - \frac{2}{3}\nabla \cdot \vec{v} I\right] \tag{4}$$

The term μ represents the molecular viscosity, while I is the unit tensor, and T represents temperature.

The turbulence model adopted in the pipe flow model is the standard $k-\varepsilon$ model. The two-equation turbulence model is broadly employed in different engineering applications due to its accuracy and quick convergence rate. In the $k-\varepsilon$ model, k represents the turbulence kinetic energy, while ε represents the dissipation rate. The standard $k-\varepsilon$ model assumes a fully developed turbulent flow, which is the setup of the pipe flow system simulated in this study. The near wall flow function selected in the models is the same scalable wall function described in Cadorin et al. [7].

The Redlich–Kwong equation of state (EOS) was selected for simulating the gas mixture properties in the models because Cadorin et al. found that the Redlich–Kwong EOS provides a proper estimation of the fluid density and dynamic viscosity [7]. These two properties along with other physical properties of hydrogen and methane can be comparably defined using the Redlich–Kwong EOS in FLUENT.

CFD modeling

A CFD model that predicts the flow behavior of a hydrogen-methane blend with 10 volume % hydrogen is first constructed and validated with the results of a reference model,

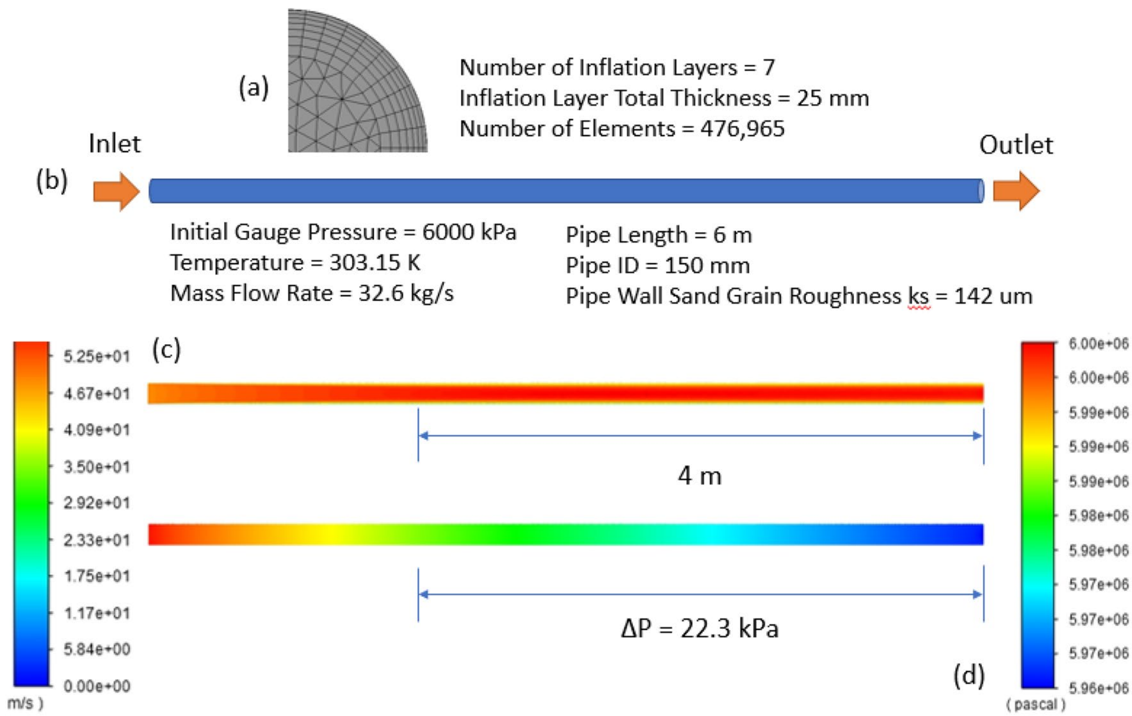

Fig. 1 Reference model **a** mesh diagram, **b** geometry and boundary conditions, **c** velocity contours, **d** pressure contours

using the same geometry, boundary conditions, and numerical methods as described in Cadorin et al. [7].

The geometry of the reference model is a 6-m cylindrical pipe with an inner diameter (ID) of 150 mm (Fig. 1). The mass flow rate of the transporting gas mixture in the pipe is 32.6 kg/s, which generated a turbulence flow in the previous study. The value of sand grain roughness ($ks = 142$ µm) is used to define the inner surface roughness of pipes. It is based on Schlichting's equivalent sand grain roughness model in which any rough surface geometry can be viewed as different size of sands glued to the surface [8]. The initial gauge pressure of the system is 6000 kPa, and the operating temperature is 303.15 K. A total of 476,965 mesh elements with average element size of 12 mm are utilized to build the geometry. Inflation is used to refine the near wall region of the mesh. A total of 7 inflation layers are included in the meshed geometry and total inflation layer thickness is 25 mm. (Refining the mesh to increase the number of elements by a factor of two did not change the results of the simulations in a significant manner.)

The pressure drop results are taken from the last 4 m of the pipe to avoid the unestablished flow domain near the inlet section. Figure 1c and d illustrate the velocity and pressure results of the 6-m pipe model. It can be observed in the velocity contours, that the velocity profile near the inlet is a bit less uniform than the rest of the pipe. In the pressure contours, the overall pressure in the pipe is gradually reduced, moving from 6000 kPa at the inlet to 5960 kPa near the outlet. The last 4-m section of the pipe away from the outlet is a fair representation of the developed gas turbulence flow pattern. It was also observed that the variation of the pressure drop was linear with flow distance.

In Table 1, the modeling results of the reference case have been compared with the identical case from the Cadorin et al. study. The pressure drop result of the reference model agrees with the value found in the Cadorin et al. study with a 0.9% difference. The expressions used to calculate the numerical friction factor (f_N) and the energy specific toll (EST) are presented in Eqs. 5 and 6 [7]. In Eq. 5, p_1 and p_2 represent the pressure at measuring point 1 and 2 respectively. The term A is the pipe cross section area, while Δx is equivalent to the length L in Eq. 6.

$$f_N = \frac{2(p_1 - p_2)D}{\rho \Delta x V_1^2} = -2\rho D \frac{\Delta p}{\Delta x} \frac{A^2}{\dot{m}^2} \quad (5)$$

$$\text{EST} = \frac{(\Delta p/\rho)}{\text{LHV}} \cdot \frac{1}{L} \quad (6)$$

The energy specific toll (EST) provides a measure of the energy required to transport a fuel gas to offset pressure drops (Δp), relative to its inherent energy (i.e., the lower heating value (LHV)), per unit length of a pipeline. (D pipe diameter, V_1 inlet velocity, $\dot{m}$ mass flow rate, ρ density of gas

Table 1 Reference case results (with $k-\varepsilon$, $k-\Omega$ and $k-\Omega$ SST CFD turbulence models) compared to results of Cadorin et al. for 90/10 (vol%) CH_4/H_2 blend case

		Cadorin et al. (10% H_2)	Reference Case $k-\varepsilon$ (10% H_2)	Reference Case $k-\Omega$ (10% H_2)	Reference Case SST (10% H_2)	Cadorin et al. (NG)	Model Case $k-\varepsilon$ (NG)	Experimental Data (NG)
$\dot{m}$	[kg/s]	32.6	32.6	32.6	32.6	32.6	32.6	31.8
p	[kPa]	6000	6000	6000	6000	6000	6000	6718
T	[K]	303.15	303.15	303.15	303.15	303.15	303.15	309.1
ρ	[kg/m^3]	39.3	38.5	38.4	38.2	55.6	55.6	58.12
μ	[Pa s]	1.33×10^{-5}	1.22×10^{-5} [9]	1.22×10^{-5}	1.22×10^{-5}	1.38×10^{-5}	1.38×10^{-5}	1.27×10^{-5}
LHV	[KJ/kg]	49,258	50,186 [10]	50,186	50,186	47,351	47,351	–
Re	[–]	2.09×10^{7}	2.31×10^{7}	2.30×10^{7}	2.29×10^{7}	2.00×10^{7}	2.01×10^{7}	2.00×10^{7}
Δp	[kPa]	22.1	22.3	22.8	23.3	15.5	15.7	–
L	[m]	4	4	4	4	4	4	–
f_N	[–]	1.91×10^{-2}	1.89×10^{-2}	1.93×10^{-2}	1.96×10^{-2}	1.90×10^{-2}	1.92×10^{-2}	2.05×10^{-2}
EST	[m^{-1}]	2.86×10^{-6}	2.89×10^{-6}	2.96×10^{-6}	3.04×10^{-6}	1.47×10^{-6}	1.49×10^{-6}	–

The results of the reference model (with $k-\varepsilon$ turbulence model) is also compared to the results of Cadorin et al. [7] and experiments for natural gas (NG) case

and L length of pipeline) Higher EST value would indicate that a greater amount of energy is required for transportation.

By comparing the results obtained from the CFD simulations of the present study using the $k-\varepsilon$, $k-\boldsymbol{\Omega}$ and $k-\boldsymbol{\Omega}$ SST turbulence models for the gas blends with 10% H_2, with those obtained by Cadorin et al. it is evident that there is no significant difference in the predictions for the pressure drops, friction factor and EST values (Table 1). Furthermore, the results of the CFD simulations using the $k-\varepsilon$ model are also compared to the experimental results obtained from a study of the flow behavior of natural gas and the simulations conducted by Cadorin et al. and good agreement with the friction factors is obtained (Table 1).

Thus, the reference case (with $k-\varepsilon$ turbulence model) is considered as a valid model that simulates the methane-hydrogen gas mixture flow in a horizontal straight pipe. The reference model is then treated as a base model for further investigations of factors that influence the energy costs associated with the transport of several blends of methane-hydrogen mixtures under different pipeline operating conditions.

Effects of hydrogen concentration and flow boundary conditions

Six CFD models, each with different methane-hydrogen concentration volume ratios (100/0, 90/10, 75/25, 50/50, 25/75, 0/100) were constructed using the same geometric configuration as in the reference model. To assess the energy costs associated with the transport of a variety of gas blends, four types of boundary conditions that mimic four potential pipeline flow conditions were imposed in the simulations—constant mass flow rate, constant inlet volumetric flow rate, constant energy flow rate at relatively lower inlet pressures and constant energy flow rate at higher inlet pressures. Thus, for each gas or gas blend, the flow behavior was captured for four distinct flow boundary conditions.

The Reynolds numbers calculated from the velocity results obtained in all the cases suggest that turbulence flows are maintained in each case. The LHV of each gas mixture was referenced and interpolated from Flekiewicz and Kubica [10]. The EST and f_N values were calculated based on the pressure drop values extracted from the CFD models of each load case. The results of the simulations, from the constant mass flow rate conditions, are summarized in Table 2. It can be observed in the table that, in general, the frictional losses generally increases as the hydrogen content increases in the gas mixtures and then drops to a lower value in the case of pure hydrogen.

By invoking the EST metric, a measure of the energy costs associated with the transport of various blends of gases can be obtained. In general, an increase in the energy costs is expected when hydrogen, with its lower density, is transported along with methane (which has higher density) in various blend ratios. However, the amount of increase in energy costs depends on the volume fraction of hydrogen and the nature of the flow conditions (Fig. 2).

Among hydrogen-rich blends, the lowest energy costs are projected for transporting pure hydrogen under the conditions where the inlet velocity flow rates are similar to that of pure methane. This type of flow conditions may be expected in the field where industrial users expect a certain amount of energy content to be delivered but are not sensitive to the rate at which that energy is delivered.

Among hydrogen-lean blends, lower energy costs are also projected for the case where pure hydrogen is transported with a mass flow rate that is proportionally adjusted to be

Table 2 Results of hydrogen concentration study with constant mass flow rate

		Methane/hydrogen Vol. % ratio					
		100/0	90/10	75/25	50/50	25/75	0/100
$\dot{m}$	[kg/s]	32.6	32.6	32.6	32.6	32.6	32.6
p	[kPa]	6000	6000	6000	6000	6000	6000
T	[K]	303.15	303.15	303.15	303.15	303.15	303.15
ρ	[kg/m^3]	42.1	38.5	30.8	24.5	14.1	4.58
μ	[Pa s]	1.26×10^{-5}	1.22×10^{-5}	1.15×10^{-5}	1.10×10^{-5}	1.00×10^{-5}	9.15×10^{-5}
LHV	[KJ/kg]	50,050	50,186	50,365	50,980	53,008	119,900
Re	[-]	2.20×10^{7}	2.31×10^{7}	2.34×10^{7}	2.79×10^{7}	2.99×10^{7}	2.95×10^{7}
Δp	[kPa]	21.0	22.3	30.9	59.8	149.8	215.8
L	[m]	4	4	4	4	4	4
f_N	[−]	1.95×10^{-2}	1.89×10^{-2}	2.10×10^{-2}	3.23×10^{-2}	4.65×10^{-2}	2.18×10^{-2}
EST	[m^{-1}]	2.50×10^{-6}	2.89×10^{-6}	4.98×10^{-6}	1.20×10^{-5}	5.01×10^{-5}	9.82×10^{-5}

similar to that of pure methane, but at a pressure that is higher than that of methane. The relationship for the energy flow rate that is used to calculate the appropriate mass flow rate for a gas blend which takes into account the LHV of the gas blend is given below:

$$\dot{E} = \mathrm{LHV}_1 \cdot \dot{m}_1 = \mathrm{LHV}_2 \cdot \dot{m}_2 \quad (7)$$

In Eq. 7, the subscripts ‘1’ and ‘2’ represent two gas blends 1 and 2 with different hydrogen volume fractions. This type of flow conditions may be expected in situations where the users expect a certain amount of energy content to be delivered at the same rate at which it is delivered in the case of pure methane. However, under conditions of constant energy flow rates, if the inlet pressure conditions for transporting gas blends are maintained similar to that of methane, then the energy costs are expected to be higher.

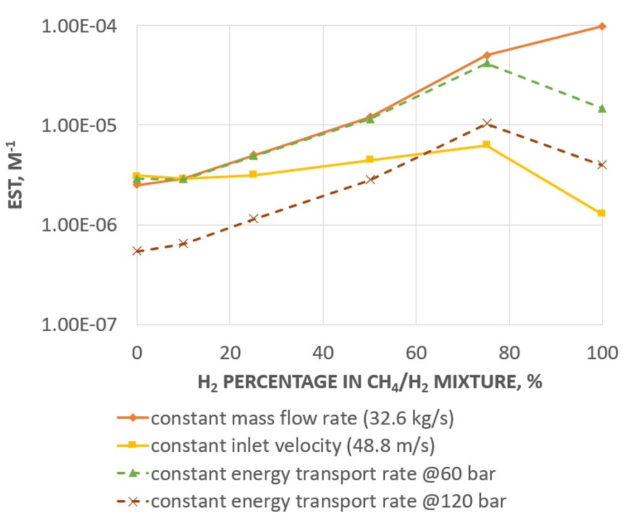

Fig. 2 Energy costs (EST) for transporting hydrogen in methane-hydrogen mixtures. (For the constant energy transport case the mass flow rate (32.6 kg/s) and LHV (50,050 kJ/kg) of pure methane is used as a baseline. The corresponding mass flow rates of various blends are obtained using Eq. 7 with the appropriate value of LHV for the corresponding blends)

Among all the gas blends of hydrogen considered in this study, the highest energy costs are projected for the transport of pure hydrogen at the same mass flow rate as methane. Under this set of flow conditions, given the higher LHV value for pure hydrogen, the end user can expect to receive energy at a rate that is significantly higher than in the case of pure methane.

Summary and conclusion

A CFD analysis was performed to assess the effects of hydrogen concentration and flow boundary conditions on the blended gas flow characteristics and the projected energy costs associated with the transportation of methane-hydrogen gas blends in straight horizontal pipe sections. In general, an increase in the energy costs is expected when hydrogen, with its lower density, is transported along with methane (which has higher density) in various blend ratios. However, the amount of increase in energy costs depends on the volume fraction of hydrogen and the nature of the flow conditions. For hydrogen-rich blends, the lowest energy costs are projected for transporting pure hydrogen under the conditions where the inlet velocity flow rates are similar to that of pure methane, while the highest energy costs are expected when hydrogen is transported at the same mass flow rate as methane.

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Data availability The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Conflict of interest The authors have no conflicts of interest to declare that are relevant to the content of this article.

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