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Reducing pressure valve with real gases: an integrated approach for the design

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Abstract

In the pursuit of an increasing cleaner fuel, methane represents a widely-employed solution for vehicles. The lower emissions, if compared to gasoline or diesel fuel, makes it an attractive opportunity in tackling transport-related pollution. Methane-powered vehicles are indeed often excluded from driving bans, pushing the demand for such kind of car. Methane is usually stored on board in tanks filled with pressure up to 20 MPa. The fuel injection systems for methane feeding usually work at pressure lower than 1 MPa (around 0.7 MPa). This difference demands a pressure-reducing valve to be installed to adjust the pressure and the fuel flow rate as required by the driver. This component and its design in hostile condition is the object of this study. Particularly, in automotive applications, the fluid operates not far from the critical point and therefore the behavior should be modelled with a real gas approach. In such light, it is immediate to note that, by the throttling procedure, the temperature of the gas drops. In addition to the acceleration of the flow, the Joule-Thomson effect related to the non-ideality of the fluid lowers the static temperature of the gas itself during the expansion. If this is combined with particularly cold environmental conditions, the material of the seals may fail entailing gas leakage. In this work, an integrated numerical and experimental study of methane fluid and thermodynamic conditions when passing through the valve orifice is reported. Extreme environmental conditions have been numerically tested, comparing and validating the results with experiments. The numerical simulations have been carried out with the open-source software suite OpenFOAM-v1712. The capability of real gas modelling has been extended by implementing a new thermophysical strategy based on the CoolProp set of libraries.

Keywords: Pressure reducing valve; Methane ; Real gas; CoolProp; OpenFOAM

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1. Introduction

Road transport is acknowledged to be one of the major causes of air pollution. In 2015, the transport sector contributed to the 21 % of the greenhouse emissions (without considering aviation and maritime transports)[2] and to the 40 % of the $PM_{2.5}$. Emissions need to fall by around two thirds by 2050, compared with 1990 levels, in order to meet the long-term 60 % greenhouse gas emission reduction target as set out in the 2011 Transport White Paper [12]. The engagement in reducing such source of pollution is testified by the several policies conducted by the European Union, for example improving fuel quality [5]. The fuel quality directive, requires a reduction of the greenhouse gas intensity of transport fuels by a minimum of 6% by 2020. Together with the Renewable Energy Directive [4], it also regulates the sustainability of biofuels. Among the others, the latter directive pushed researchers and industry to look into cleaner fuels to power vehicles. Nowadays, one of the most spread propellant is natural gas [3]. The lower emissions, if compared to gasoline or diesel, makes it an attractive opportunity in tackling transport-related pollution.

The employment of such fuel entails extra care from the design standpoint. Methane (or rather Compressed Natural Gas, CNG) is usually stored on board in tanks, with pressure up to 20 MPa. Such high pressure vessel is separated from the fuel injection systems by a pressure-reducing valve. This valve is required since the methane feeding system usually works at pressure lower than1 MPa (around 0.7 MPa), and thus pressure needs to be reduced. This operation is done by regulating the orifice height (that is related to the piston lift) to let the nozzle working between the two pressure values and allowing a certain amount of fuel flow rate as required by the driver. The valve and its design in hostile condition is the object of this study. Particularly, the design of the pressure reducing valve entails several difficulties. The flow through the orifice should entail the careful estimation of the passage area, in order to correctly predict the flow rate; typical working conditions locate the properties of the gas not far from the critical point. The real gas behaviour should be therefore taken into account, as well as the variation of the thermophysical properties. Eventually, particular severe conditions, such as very low environment temperature or very high storage pressure, can cause the fluid condensation.

In order to improve the knowledge of the behaviour of the fluid inside the nozzle, the computational fluid dynamics (CFD) can be of help. Flows through nozzles are widely studied, also when real gases are of concern, see for example [10, 11]. An example of the effects of the real gas is an upwind displacement of the shock structures, with the consequent variations in the heat transfer. Normally, the real gas modeling entails the adoption of a cubic-type laws for the modeling, so called since they can be re-written as a function of V_m^3, where V_m is the molar volume [6]. The termophysical properties as c_p or c_v and the transport properties as μ or κ are not constant but are considered as a function of the temperature. Seldom the effects of the pressure variation are considered: the pressure ratio in this nozzle, when the tank is filled, can exceed the value of 25, entailing strong variation in the thermophysical properties. For example, passing from a value of p_0=20 MPa and T_0 = 250 K to p_1=0.7 MPa and T_1 = 250 K, one finds $c_{p,0}$= 4.129 kJ/kgK and $c_{p,1}$= 2.203 kJ/kgK [7]. This is only an example of how pressure can affect the CFD reliability.

The design of the valve is particularly critical when the device operates in hostile conditions. When the engine operates,the throttling procedure causes the temperature of the gas to drop. In addition to the acceleration of the flow, the Joule-Thomson effect related to the non-ideality of the fluid lowers the static temperature ofthe gas itself during the expansion. If this is combined with particularly cold environmental conditions, the material of the seals may fail entailing gas leakage. The study of this problem is the object of this work, in order to understand how the fluid-dynamics of the fuel affects the valve temperature and the best heating strategy to avoid seals failure. The numerical simulations have been carried out with the open-source software suite OpenFOAM-v1712. The capability of real gas modelling has been extended by implementing a new thermophysical strategy based on the CoolProp set of libraries.

2. Design and Integration with CFD

The common practice when dealing with convergent-divergent nozzle and, particularly, with reduced valves, is to start with a monodimensional design. In this phase the throat area of the nozzle is to be designed starting from the pressure in the tank and at the injectors, to obtain the desired mass flow rate. The study was conducted on an existing geometry. For the CFD analyses, since the focus of this study is the throttling zone, the starting geometry has been simplified in order to consider only this particular. The inlet and the outlet of the domain are distanced from the nozzle in order not to introduce spurious effects.

Nomenclature

A	passage Area	κ	conductivity
CNG	Compressed Natural Gas	m	molecular mass
C_m	mass flow parameter	L	axial nozzle length
c_p	specific heat at constant pressure	p	pressure
C_q	flow coefficient	s	axial coordinate
c_v	specific heat at constant volume	x	valve lift
JT	Joule-Thomson	T	temperature
Greek symbols		Subscripts	
μ	viscosity	0	relative to inlet reservoir/ total quantity

2.1. One dimensional design

To adjust the nozzle throat area, the piston is moved towards to (or away from) the upper wall of the orifice: the mass flow rate to the injectors is therefore a function of the piston lift, as shown in Figure 1a. To determine the passage section as a function of the desired flow rate, one must solve $A = \dot{m}\sqrt{T_0}/C_m C_q p_0$, where C_m is the mass flow parameter and C_q is the flow coefficient. Such parameters keep into account the flow conditions and the vena contracta effect of the flow through the orifice. Particularly, according to [9], C_m is function of the fluid properties (e.g. specific heat ratio across the nozzle) and the physical state of the system (pressure ratio across the nozzle). In the case analyzed in this work, the nozzle is always chocked. Therefore, all the parameters of the former equation except the flow coefficient C_q can be assessed using explicit functions or measurements. To predict the value of C_q, the Perry's equation can be used [14]. Once the passage area is obtained, the lift of the piston and thus the orifice can be easily computed (the passage area is a cylinder of height x).

The real gas behaviour of the CNG in the nozzle can be predicted reasonably well by correcting the value of C_m with the thermophysical properties calculated according to the temperature and pressure. Referring to an ideal-gas, quasi-one dimensional nozzle analysis for a guideline on the flow structures, the pattern is as reported in Fig. 1b. What it is difficult to be correctly predicted is the temperature downstream the gap, before the shock wave. This is indeed the minimum temperature of the entire domain, and it is the one that must be monitored in order to preserve the seals integrity. The static temperature trend, read on the right axis of Fig. 1b, decreases up to the shock location, due to the transformation into dynamic temperature. This phenomenon is the only responsible of the temperature decrease for ideal gases. On the other hand, for real gases, the compressibility factor different from 1 entails the Joule-Thomson (JT) effect [15]: an isoenthalpic throttling causes an extra variation of the temperature, that can both increase or decrease, depending on the conditions. For CNG in storage-like conditions, both experimentally and from the literature, the temperature undergoes an extra drop.

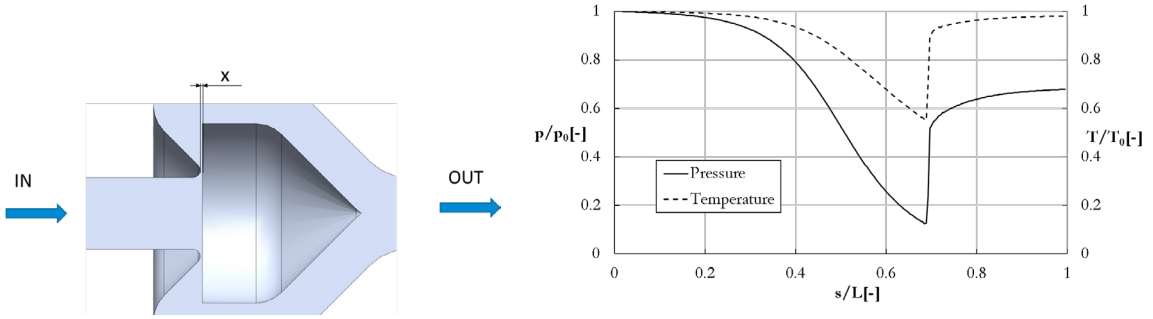
The temperature drop related to both flow acceleration and JT lamination, poses a real hazard for valve sealants, entailing leakages. To avoid such danger, a heating system is installed, recirculating engine cooling water as a heat source for the CNG. It is well clear that the resulting flow and temperature field is almost impossible to be correctly predicted by a one-dimensional analysis. A CFD simulation should be set-up for trying to consider all these contributions.

2.2. CFD

2.2.1. Ideal gas approach

The valve was firstly analyzed by modeling the fluid under the ideal gas approach, in order to investigate the potentialities of such approach. The boundary conditions applied for this computation are reported in Tab. 1

The compressible solver *rhoPimpleFoam* was employed with the ideal gas law. The computation run on a slice of the axi-symmetric valve, with structured hexa grid as reported in Fig. 2. The turbulent model employed is a High-Re k-ε, with standard wall functions. The thermophysical properties (c_p, μ and κ) in this very first approach were



(a) Particular of the nozzle area: the piston lift x determines the throat section

(b) Normalized static pressure and temperature in a quasi one dimensional nozzle flow

Fig. 1: Geometry of the nozzle and analytical solution for a quasi-one dimensional nozzle

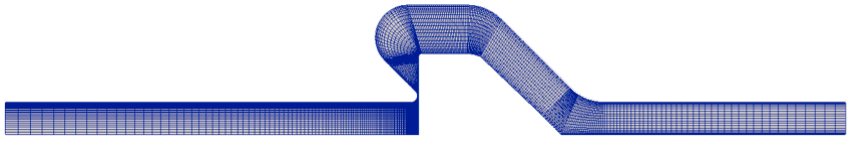


Fig. 2: Grid used for the computation.

considered constant and are evaluated at a pressure that is intermediate in the range of values assumed by the gas. Under these hypotheses, the temperature distribution in the domain is the one reported in Fig. 3.

Having the inlet on the right hand side, the flow enters the domain at high pressure and temperature. The temperature remains constant in this area. Approaching the gap, the fluid accelerates in the convergent part of the orifice. The velocity keeps increasing (due to the associate decrease of pressure) in the divergent part up to the shock wave. This pattern is in agreement with what expected from Fig. 1b. The temperature is therefore very low just upstream the shock, but the recovery after the shock is such that the value is almost equal to the inlet one. This result is expected, as a direct consequence of the total enthalpy conservation with constant c_p and adiabatic wall (no heat is supplied in this case). Unfortunately, experimental data report a drop in temperature at the outlet, that is not correctly reproduced by the numerical model. Nonetheless it is interesting to evaluate the fact that the conditions of pressure and temperature just before the shock are such that condensation might be expected in the actual test.

2.3. Real Gas approach

The ideal gas approach has severe limitations, as above reported. It is therefore necessary to pass to a more complex level of modeling, and to employ the real gas approach. The real gas model, together with a non-constant value of thermophysical and transport properties, may help in obtaining a more reliable numerical model. In light of this, the

Table 1: Boundary conditions for the ideal gas computation

	Quantity	Value
Inlet	p_0	10.1 MPa
	T	248 K
	Turbulence intensity	1.00 %
	Turbulence mixing length	0.000121 m
Wall	T	adiabatic
Outlet	p	0.80 MPa

Peng-Robinson model [13] that comes with the software has been used. This model requires the properties of the fluid at the critical point and the acentric factor ω. This is related to the fact that in correspondence to the critical point, the derivatives of the pressure with respect to the volume vanish [13] and thus the EOS can be solved. The critical properties of the methane have been used, introducing an approximation on the natural gas composition [8]: the typical methane content is around 95 %, but it is dependent on the supply. The properties used are therefore: $R = 518.46 J/kgK$, $m = 16.04 kg/kmol$, $T_{crit} = 191 K$, $p_{crit} = 4.6 MPa$ and $\omega = 0.01$.

For what concerns the variation of the other properties with the temperature, a polynomial expression was chosen for all of them. Particularly, in this step, the properties were evaluated at a reference pressure of 5 MPa. The variation of the c_p with the temperature is reported in Fig. 4 to show how these properties are affected from the temperature. A variation that exceeds the 50 % spanning the temperature range covered by the methane in the current application is reported. In Fig. 4, the polynomial expression used in this work is reported. It can be seen that a forth-order polynomial represents well the c_p variation. The temperature pattern resulting from such computation is reported in Fig. 5.

With respect to the ideal gas computation, there is basically no difference in the temperature distribution up to the orifice. The acceleration downstream the gap is such that the minimum temperature inside the domain is slightly higher than the ideal gas analysis. This is related with a lower Mach number just before the shock (that is sligthly displaced upstream), which finds good agreement in the literature [11]. The major differences with respect to the former case are downstream the shock. The real gas approach allows a lower temperature to be reached downstream the orifice.

Quantitatively speaking, the current set-up leads to a reduction of the outlet temperature up to a value of 215 K. A theoretical JT expansion would lead to an outlet temperature of 185 K. The difference with this theoretical value is thought to be related to the variation of thermophysical properties with the pressure also, since the real gas model has been proved to be accurate in the prediction of the compressibility factor [13]. An extra change should be introduced for trying to cover the 30 K of difference between the actual and the theoretical value of the outlet temperature.

2.4. Real gas approach with pressure effect on the thermophysical properties

To bridge the gap in outlet temperature, the pressure effect on the properties has been introduced. This feature is usually available in CFD software by computing the departure quantities thanks to the real gas model. Few of them allow the usage of lookup-tables to be filled with a-priori calculated properties. The method developed in this work, allows the runtime computation of the properties in the current state. This is done by implementing the open-source library CoolProp [1] into OpenFOAM-v1712. Every time the solver requires for the computation of the thermophysical properties, the library is called. This happen several times per iteration since a Newton's iterative technique is employed for finding the value of such properties. This library has been used to evaluate c_p, μ and κ, whereas for the density, the Peng-Robinson model has been employed.

By using this approach an issue arises. Particularly, in the above explained methods, the phase change was not considered at all. Even if the physical properties at some point of the valve where such that condensation may have occurred, the solver is not aware of such transformation: the polynomials used are continuous, ensuring robustness to the simulation, but preventing the second phase inception. CoolProp, and thus the current approach, returns for the

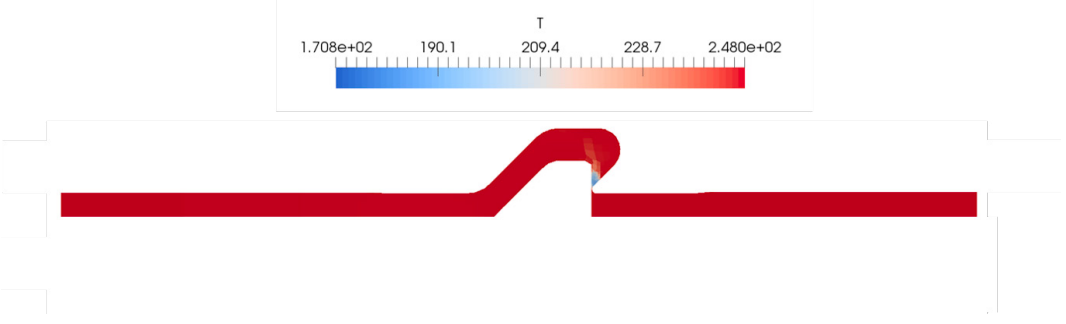


Fig. 3: Temperature pattern of the CNG inside the valve under the ideal gas assumption

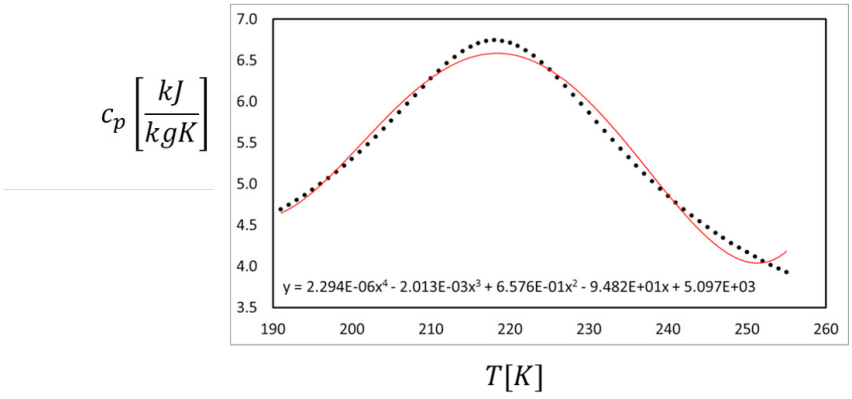


Fig. 4: Variation of c_p with the temperature at a reference pressure of 5 MPa

state the actual properties that may be relative to the liquid phase, if the conditions are such that condensation happen. This entails a step-wise variation of the properties that may cause a trouble in the Newton-like iterative technique above mentioned. Indeed, simulations run with this approach are highly unstable, preventing to achieve convergence. This is related to the fact that a single-phase solver was used, that cannot keep into account liquids if the carrier phase is gaseous and vice-versa. The employment of this type of solver is considered the next step of this work.

In order to prevent condensation to arise, a numerical trick has been introduced. To prevent the physical state of the gas to go below the saturation curve, the thermophysical properties are evaluated as a linear interpolation between the one predicted by CoolProp and the polynomial expression suggested in 2.3. In other words, the final value of the thermophysical properties are:

$$c_p = \alpha_{c_p}\, c_{p,CoolProp(f(p,T))} + (1 - \alpha_{c_p})\,(c_{p,poly(f(T))}) \tag{1}$$

where the blend coefficients α_i are such that the closer to 1 they are, the closer the i property will be to the CoolProp prediction. On the other hand, $\alpha_i \to 0$ improves stability. For μ and κ the same expression ahave been used.

This introduces a simplification of the problem leading to an approximation of the flow field. The different thermophysical properties of the liquid with respect to the gas and the latent heat of vaporization are not considered as well as the presence of an interface among the two phases. Nonetheless, the results in terms of temperature distribution obtained with the current approach is very close to the one predicted by the JT effect, as reported in Fig. 6. Specifically, employing $\alpha = 0.6$ for all the (1), the outlet temperature is equal to 188.5 K, when the JT effect was equal to 185 K

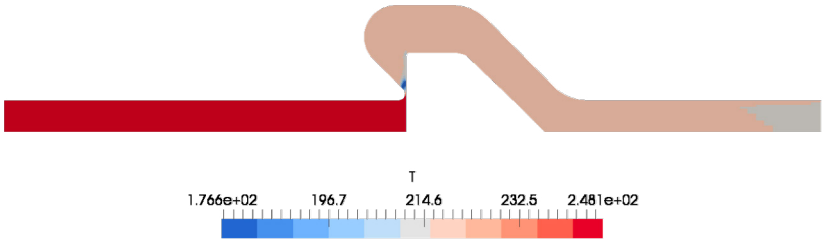


Fig. 5: Temperature pattern when the real gas model and the variation of thermophysical and transport properties with the temperature are considered.

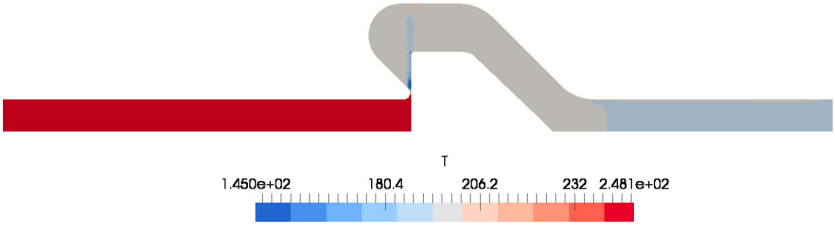


Fig. 6: Temperature pattern when the real gas model and the variation of thermophysical and transport properties with both temperature and pressure are considered

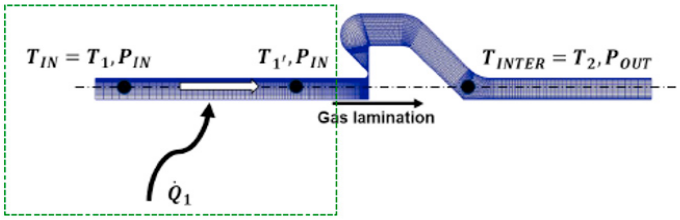


Fig. 7: Schematic for the heat transfer evaluation

(with a difference in the predicted temperature of the 2 %). This close value, even if the condensation is not modeled, may be explained under two different standpoints. First, the area where the condensation happen (that should be visualized as a quite thin curtain of small liquid droplets just before the shock), may be very small not having a major effect on the overall flow from the standpoint of the temperature pattern. On the other hand, the latent heat released when the gas liquefies, is re-adsorbed (even if in different conditions) when the liquid vaporizes back. The balance of the two changes of phase might be such that the overall result is quite accurate. This guess of course does not hold when the heat transfer is to be accurately evaluate in the orifice area. In spite of this, it makes the results presented here a reasonable starting point for the design considerations.

2.5. Heat transfer analysis

As above mentioned, the need for the numerical model is devoted to predict the heat to be supplied and the optimal position to locate the heating source (i.e. the engine-cooling water). Given the results shown in the previous paragraph, since the nozzle is chocked, the only possible location where to supply the heat is upstream the orifice. Since the heat to be supplied to the CNG is concentrated upstream the gap, the lamination may be considered as adiabatic. If the lamination is adiabatic (and thus isoenthalpic), the transformation should be a JT expansion. In light of this, the amount $\dot{Q}$ to be transferred to the fluid is the one that predicts an upstream temperature $T_{1'}$ such that a JT lamination from that temperature would entail an outlet temperature equal to the experimental one, as sketched in Fig. 7. This assumption is to be introduced since even if an experimental apparatus would be available, it is difficult to evaluate the amount of heat supplied by the sorrounding environment.

In light of these considerations, an experimental test-bench was set up with the help of Metatron S.p.A. The pressure reducing valve, having the same geometry in the nozzle area, was tested under the same conditions proposed in this work. The outlet temperature experimentally found was -61.5°C. With the considerations summed up in Fig. 7, the amount of heat to be transferred is calculated through $\dot{Q} = \dot{m}(h_{1'} - h_1)$. The heat is indeed supplied in an isobaric process.

Given an inlet temperature T_1 of -25°C, $T_{1'}$ has been found to be equal to -13.8°C, to return an outlet temperature $T_2 = -110$°C . The total thermal power to be supplied is therefore $\dot{Q} = 155$ W, the theoretical JT expansion predicts -143°C. By supplying the power calculated as above, in the numerical calculation, an outlet temperature of -85°C was found, with a difference of 23.5°C with the experimental value, with an error of approximately 20%. The difference

in the prediction might be related to two main facts. In the assumption presented in this section, the heat is supplied at constant c_p to raise the temperature to the value needed for an "equivalent" JT lamination. Experimentally, the heat is transferred by the body of the valve. This means that heat is supplied both upstream, downstream and in the orifice area: the fluid has different c_p in these sections, and thus the increase in temperature for a given amount of heat transferred is different. For example at p=200 bar and T= -25° C, c_p=4.1376 J/kgK but if p=8 bar and T= -110°C, representing the outlet conditions of the experimental test, c_p=2.35 J/kgK. On the other hand there might be presence of condensation in the orifice: the variation of the thermophysical properties when the walls are not adiabatic may be responsible for the mismatch of the prediction. A two-phase computation is probably more suitable for solving this problem.

3. Conclusion

In this work a numerical model to simulate the behaviour of the CNG inside a pressure reducing valve is set-up. The procedure has been developed keeping an eye towards the integration with the design process. Particularly, a robust thermophysical model that involve the computation of properties with the aid of CoolProp library has been carried out. Besides, a blend factor to allow not to consider the second-phase inception due to condensation has been introduced. Preliminary results show good agreement with the theoretical values, but more work has to be devoted for the accurate and a-priori estimation of the heat transfer. The next steps in this track are the switching to a two-phase calculation and the study of how to more effectively transfer the heat to the flow field.

Acknowledgements

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References

[1] Bell, I.H., Wronski, J., Quoilin, S., Lemort, V., 2014. Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library coolprop. Industrial & Engineering Chemistry Research 53, 2498–2508. URL: http://pubs.acs.org/doi/abs/10.1021/ie4033999, doi:10.1021/ie4033999, arXiv:http://pubs.acs.org/doi/pdf/10.1021/ie4033999.

[2] EEA, 2015. Greenhouse gas emissions from transport. https://www.eea.europa.eu/data-and-maps/indicators/transport-emissions-of-greenhouse-gases/transport-emissions-of-greenhouse-gases-10. Accessed: 24-05-2018.

[3] Engerer, H., Horn, M., 2010. Natural gas vehicles: An option for europe. Energy Policy 38, 1017–1029.

[4] European Commission, 2009a. Directive 2009/28/EC of the European Parliament and of the Council of 23 April 2009 on the promotion of the use of energy from renewable sources and amending and subsequently repealing Directives 2001/77/EC and 2003/30/EC (Text with EEA relevance). Technical Report.

[5] European Commission, 2009b. Directive 2009/30/EC of the European Parliament and of the Council of 23 April 2009 amending Directive 98/70/EC as regards the specification of petrol, diesel and gas-oil and introducing a mechanism to monitor and reduce greenhouse gas emissions and amending Council Directive 1999/32/EC as regards the specification of fuel used by inland waterway vessels and repealing Directive 93/12/EEC (Text with EEA relevance). Technical Report.

[6] Fishbane, P.M., Gasiorowicz, S.G., Thornton, S.T., 2005. Physics. Prentice-Hall.

[7] Friend, D.G., Ely, J.F., Ingham, H., 1989. Thermophysical properties of methane. Journal of Physical and Chemical Reference Data 18, 583–638.

[8] Gandhidasan, P., Ertas, A., Anderson, E., 1991. Review of methanol and compressed natural gas (cng) as alternative for transportation fuels. Journal of Energy Resources Technology;(United States) 113.

[9] ISO 6358-3:2014, 2014. Pneumatic fluid power – Determination of flow-rate characteristics of components using compressible fluids – Part 3: Method for calculating steady-state flow-rate characteristics of systems. Standard. International Organization for Standardization. Geneva, CH.

[10] Jassim, E., Abdi, M.A., Muzychka, Y., 2008a. Computational fluid dynamics study for flow of natural gas through high-pressure supersonic nozzles: Part 1. real gas effects and shockwave. Petroleum Science and Technology 26, 1757–1772.

[11] Jassim, E., Abdi, M.A., Muzychka, Y., 2008b. Computational fluid dynamics study for flow of natural gas through high-pressure supersonic nozzles: Part 2. nozzle geometry and vorticity. Petroleum Science and Technology 26, 1773–1785.

[12] for Mobility, E.C.D.G., Transport, 2011. White Paper on Transport: Roadmap to a Single European Transport Area: Towards a Competitive and Resource-efficient Transport System. Publications Office of the European Union.

[13] Peng, D.Y., Robinson, D.B., 1976. A new two-constant equation of state. Industrial & Engineering Chemistry Fundamentals 15, 59–64.

[14] Perry, J.A., 1948. Critical flow through sharp-edged orifices. Trans. A.S.M.E 71, 757.

[15] Shoemaker, D.P.G., Carl, W., et al., 1967. Experiments in physical chemistry/David P. Shoemaker y Carl W. Garland. Technical Report.