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COMPUTATIONAL SIMULATION OF FLOW IN A SUPERSONIC GAS SEPARATOR

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Abstract. *The purpose of the current study is to analyze the flow in a supersonic nozzle with the objective of better understanding of the flow in different configurations. To achieve this understanding, numerical simulations were carried out using computational fluid dynamics (CFD) in order to quickly inspect the behavior of the flow and make conclusions based on the analysis of calculated flow fields using CFD. To determine which equations of state and turbulence models to use we tested different setups and the results of each setup were compared to identify the influence of the choices. This study grounds the choice of models in the final simulations, which have the objective of studying the phenomenon of fluid separation in a multiphase flow by the introduction of a secondary flow.*

Keywords: *Supersonic, Separation, CFD, Models, Multiphase*

1. INTRODUCTION

The exploration of new oil wells by the oil industry in the pre-salt layer in Brazil created many new demands as the properties of the gas and oil presents in the wells are different from what is usually found in the post-salt reservoirs. In this new explorations some companies find out that the composition of the gas, which is mainly composed of methane, has a high concentration of carbon dioxide. As this discovery was made the way of turning the exploration of the gas in a more attractive investment was to purify it in the off-shore platforms, as this purification would reduce the costs of transportation of the gas to land. Many developments were made in this sense but the technology is still too immature to be properly explored.

A new method of gas separation that can be used in the above mentioned example the use of a supersonic gas separator. This consists in making the gas flow through a nozzle with swirl, under conditions that allows the carbon dioxide to change phase, going from gas to liquid. The state near condensation for CO2 is reached as a converging-diverging nozzle is used and it transforms the enthalpy of the fluid into kinetic energy. The decrease of enthalpy makes the temperature and pressure to drop and as supersonics conditions are reached this phenomenon is highly intensified.

As the CO_2 goes to the liquid state, it has a great increase in the specific mass. This increase makes it possible to centrifuge the CO_2 from the CH_4 as the flow is rotational. Therefore it is possible to extract the unwanted condensate components of the gas mixture. Figure 1 shows an image of a supersonic gas separator from Twister – Supersonic gas solutions company that makes it possible to better understand the process.

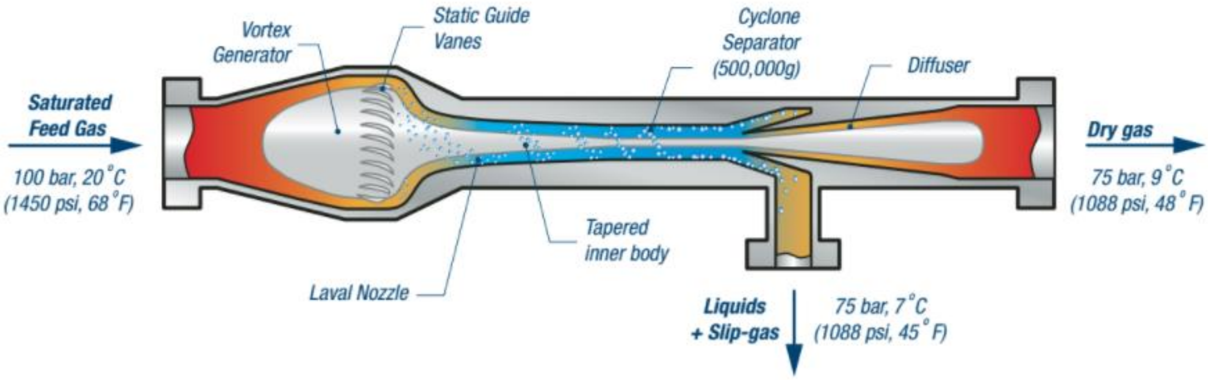

Figure 1. Cross-section of a Twister tube with typical process conditions (Twister, 2017)

Therefore, the study of flow through supersonic nozzles is very important to understand this phenomenon and because of that many researchers have been putting efforts in the determination of how the simulation parameters can influence the precision of the results. As an example, (Farag, 2013) has studied the influence of the turbulence model and mesh configuration in the study of the flow in a supersonic nozzle and (Jassim, 2008) focused his study in the evaluation of the influence of the equation of state (real and ideal gas models) in the results of simulations of the flow in a supersonic nozzle.

2. NUMERICAL SIMULATIONS

The fundamental function of the numerical simulations is to calculate momentum, energy and mass balances in the elements of the fluid mesh. Those balances are given by three main equations of the fluid mechanics that are expressed in Eqs. (1), (2) and (3).

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot \left(\rho U U\right) - \nabla \cdot \mu \nabla \cdot U = -\nabla p \tag{1}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho U\right) = 0 \tag{2}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \left(\rho U e\right) - \nabla \cdot \left(\frac{k}{C_v}\right) \nabla \cdot e = p \nabla U \tag{3}$$

Those balances are applied in the mesh elements that must be sized in a way that it is possible to capture the phenomena of the flow. So it is very important to have a previous knowledge of how the flow will work to be able to identify regions with high gradients and refine the mesh in those regions so as to make it possible to accurately determine the characteristics of the flow.

2.1 CFD Tool

As the main tool of the research, the *OpenFOAM* CFD toolkit was used to carry out the simulations of the flow inside the converging-diverging nozzle. *OpenFOAM* has many flow solvers for different applications and the most suitable transient solvers identified were *rhoPimpleFoam*, ideal to simulate compressible flow, and *twoPhaseEulerFoam*, which is highly recommended for multiphase flow of liquid and gas. Besides the presence of a wide range of solvers for many applications, there was a library of equations of state and turbulence models already implemented in the software, which made it possible to make the comparisons we intended. Two models that deserve to be highlighted are the real gas model of Peng-Robinson and the turbulence model *k-ω SST*.

The gas model of Peng-Robinson is very good at predicting the state of gases like CO_2 in wide range of conditions (Manning, 1991). This is possible as the modeling takes in account many factors related to the substance, as the a , b and α factors are functions of the critical pressure and temperature and the acentric factor, and reach the Eq. (4), which have its factors determined by Eqs. (5), (6), (7), (8) and (9).

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m^2 + 2bV_m - b^2} \tag{4}$$

$$a = \frac{0.45724\, R^2 T_C^2}{P_C} \tag{5}$$

$$b = \frac{0.07780\, R\ T_C}{P_C} \tag{6}$$

$$\alpha = (1 + \kappa(1 - \sqrt{T_r}))^2 \tag{7}$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{8}$$

$$T_r = \frac{T}{T_C} \tag{9}$$

Yet the *k-ω SST* turbulence model is a powerful model to predict accurately the flow as it uses the *k-ω* near walls, which are regions with high gradients due to viscous effects, and the *k-e* in the other regions, which have small gradients. This model makes it possible to accurately determine the effects in regions with high gradients and avoid numeric errors in low gradients regions. To formulate mathematically the *k-ω SST* model the equations of the other two models are combine giving origin the Eqs. (10) and (11) (Wilcox, 2006).

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \rho P - \beta_a \rho \omega k + \frac{\partial}{\partial x_j}[(\mu + \sigma_k \mu_t)\frac{\partial k}{\partial x_j}] \tag{10}$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \gamma P_\omega - \beta \rho \omega^2 + 2\rho(1 - F_1)\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} + \frac{\partial}{\partial x_j}[(\mu + \sigma_\omega \mu_t)\frac{\partial \omega}{\partial x_j}] \tag{11}$$

2.2 Nozzle geometry and mesh

To start the investigations about this flow we chose a geometry based on a literature review, the geometry used in the article was reconstructed and is shown in Figure 2. The article (Arina, 2004) has also theoretical predictions that were used to validate the results obtained in preliminar simulations.

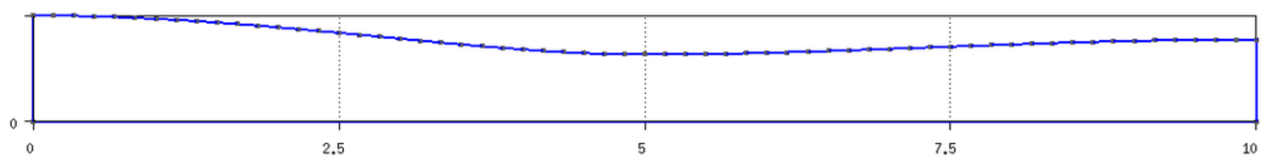

Figure 2. Profile of the geometry of study

After the determination of a geometry, we needed to specify the mesh to be used in the numerical simulations, we employed a 2D mesh of 1500 elements in the axial direction and 80 elements in the radial direction with a cell grow factor of 1.02. The simulations were axisymmetric.

3. CODE VALIDATION

In order to verify if the implemented code in the software was correct we used the conditions and results of (Arina, 2004) simulation as a reference for validation. The same boundary conditions were used as shown in Table 1 and the same fluid was used, in the specific case, air.

Table 1. Boundary conditions for validation simulation.

Magnitudes	Inlet	Outlet
Total Pressure (Pa)	101148	-
Static Pressure (Pa)	-	83048
Static Temperature (K)	288	-

After carrying out the simulation with the *rhoPimpleFoam* solver, we concluded that the results were very close. The pressure field has a great drop and a normal shock appears in the flow as shown in Figure 3. This behavior is expected for a compressible supersonic flow as can be seen in (Wylen, 1998)

Figure 3. Static pressure field in Pa of ideal and inviscid airflow using Table 1 conditions through a nozzle with the geometry of (Arina, 2004)

4. MODEL DETERMINATION

As the flow operate in extreme conditions, we needed to verify the influence of the equations of state and turbulence models while predicting the flow behavior. For this purpose many simulations were carried out with the boundary conditions of Table 2 in order to identify which was the best model to apply in the simulations. As the static temperature is one of the most important quantities the results for this field of different simulation are shown in Figure 3.

Table 2. Boundary conditions for model determination simulations.

Flow Title	Magnitudes	Inlet	Outlet
Air Inviscid; Air turbulent – Ideal gas; Air turbulent – Peng Robinson.	Total Pressure (Pa)	101148	-
	Static Pressure (Pa)	-	83048
	Static Temperature (K)	288	-
Air turbulent with rotation – Ideal gas	Total Pressure (Pa)	130000	-
	Static Pressure (Pa)	-	83048
	Static Temperature (K)	288	-
	Rotation (rpm)	1500	-
Air turbulent high pressure – Peng Robinson	Total Pressure (Pa)	10114800	-
	Static Pressure (Pa)	-	8304800
	Static Temperature (K)	288	-

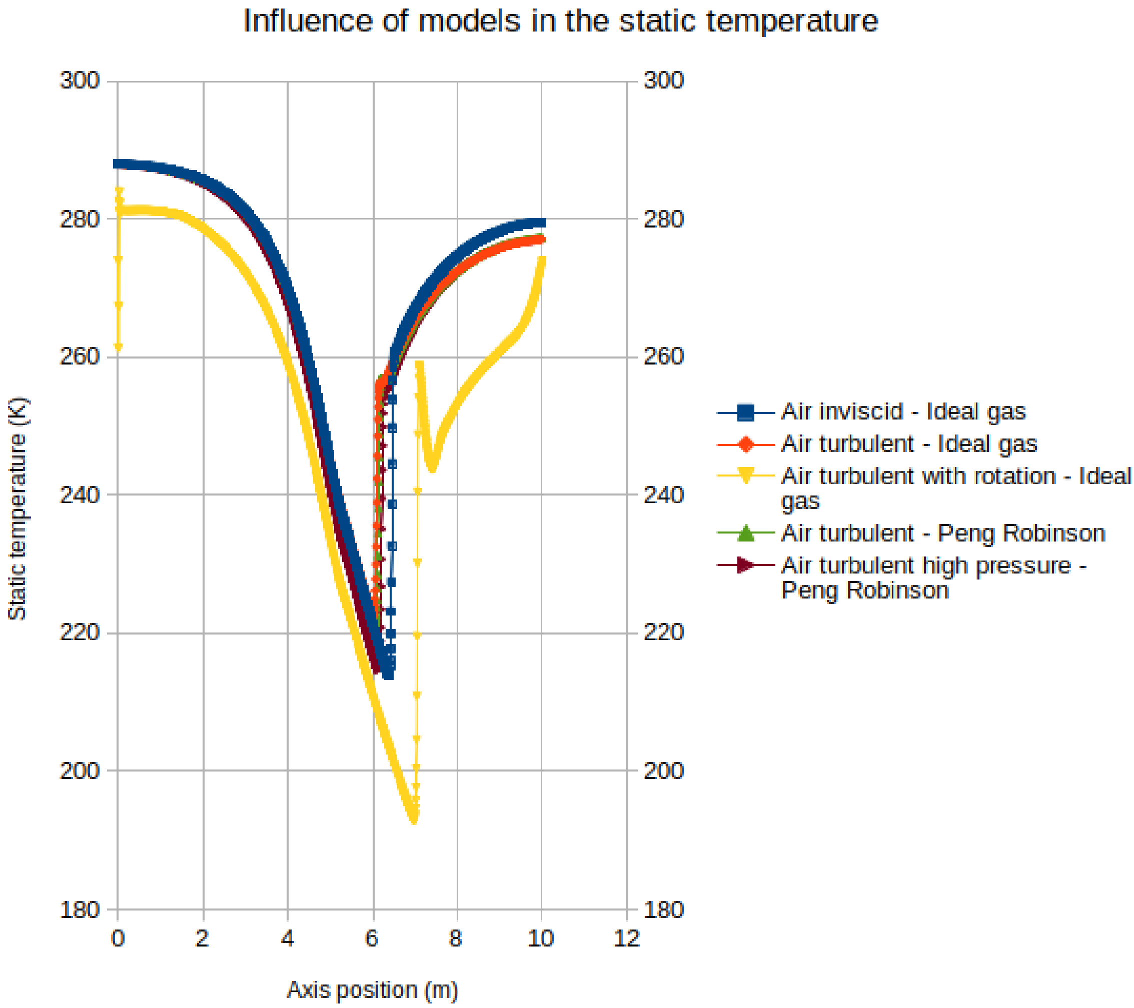

Figure 4. Graph of static temperature using different models in the simulations along the axis

With the presented results in the Figure 3, it is possible to verify that using ideal or real gas models does not make a noticeable difference in the results obtained. Other confirmation is that the presence of viscosity in the gases drags the normal shock closer to the throat, as the fluid suffers of energy loss by viscous friction.

4.1 Rotation Flow

With the addition of a secondary flow in the inlet of the nozzle, the flow fields were greatly changed. The applied boundary conditions in the simulations are in Table 2 in *Air turbulent with rotation – Ideal gas* line. As can be seen in the results presented in Figure 4 it is possible to notice that the rotation in the flow promotes the elevation of the specific mass in the peripheral region (a) comparing with the non-rotating flow (b). Because of that, there is a great drop in the axial velocity in the peripheral region (c) when comparing with the non-rotating flow (d). This increase in density can be justified, as there is a great centrifugal acceleration.

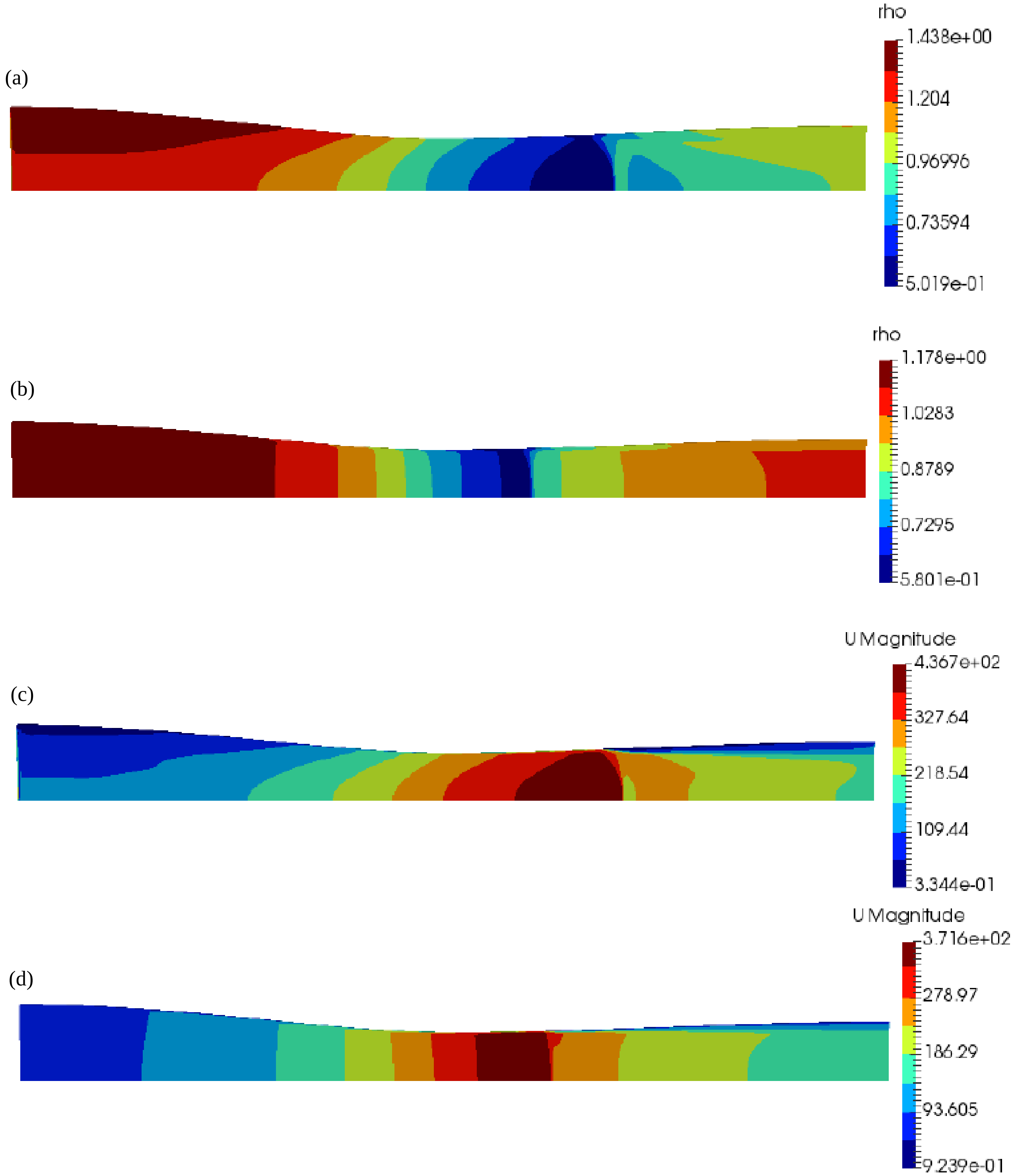

Figure 5. Comparison of specific mass an velocity fields of rotating (a, c) and non-rotating flow (b, d)

5. BICOMPONENT GAS SIMULATIONS

As the nozzle has the objective of operating with CO_2 and CH_4, simulations were carried out to verify the modifications of the flow as the gas composition is changed. The applied boundary conditions were same of Table 2 of the *Air turbulent with rotation – Ideal gas* line in the studied flows. In addition, the ideal gas model and the *k-ω SST* turbulence model were employed. The results of the simulations are presented in Figure 4 three different mixtures were employed of 30/70, 50/50 and 70/30.

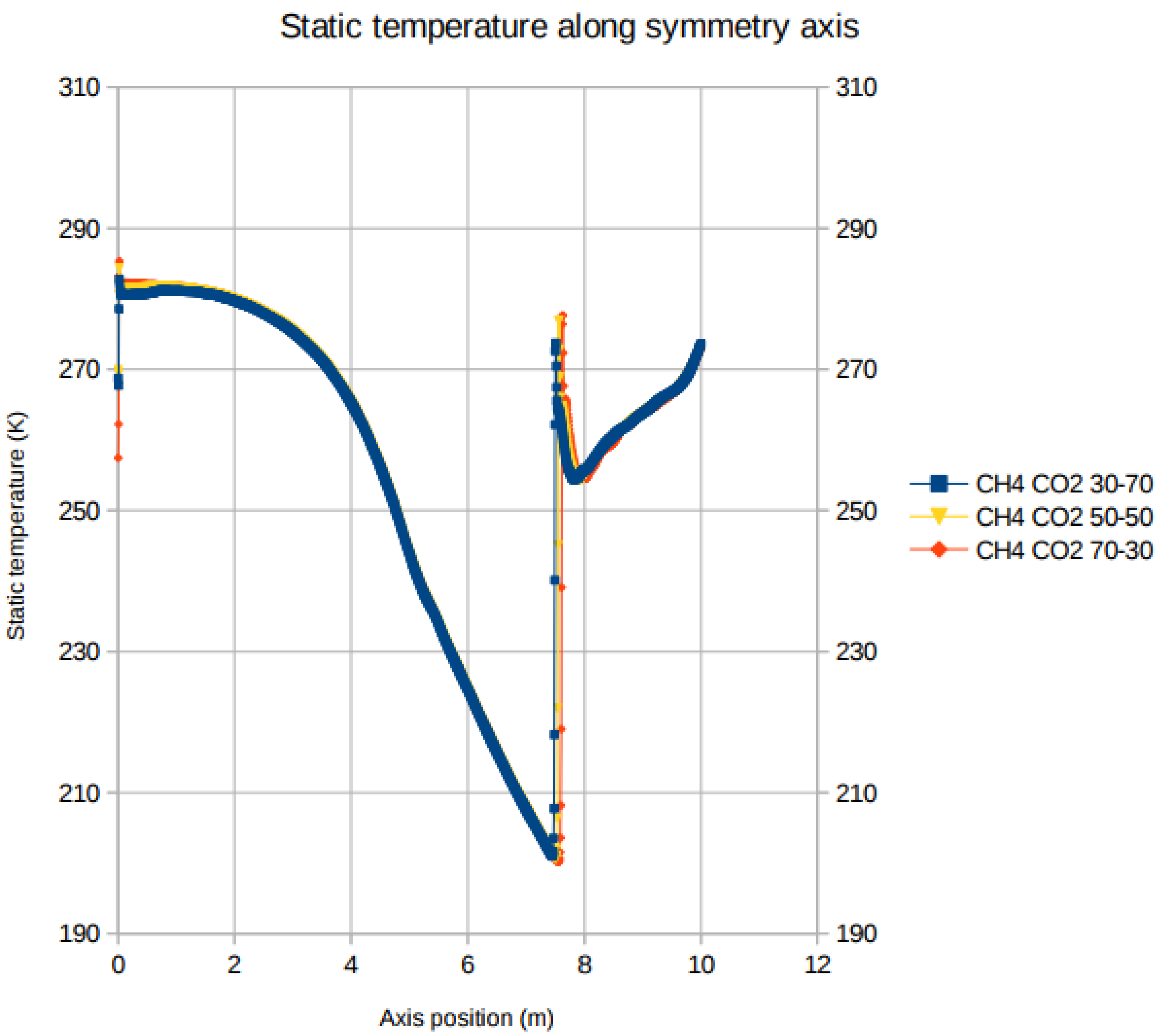

Figure 6. Comparison of static temperature along the axis of the flow with mixture at different compositions

Figure 5 shows that the flow is almost unaffected by the mixture composition change as the normal shock position did not move and the static temperature fields are almost the same. This is possibly because the specific heat ratio of the CO_2 and CH_4 are approximately the same, 1.289 and 1.299 respectively (VanWylen, 1998). The pressure field is also barely unchanged due to composition alterations.

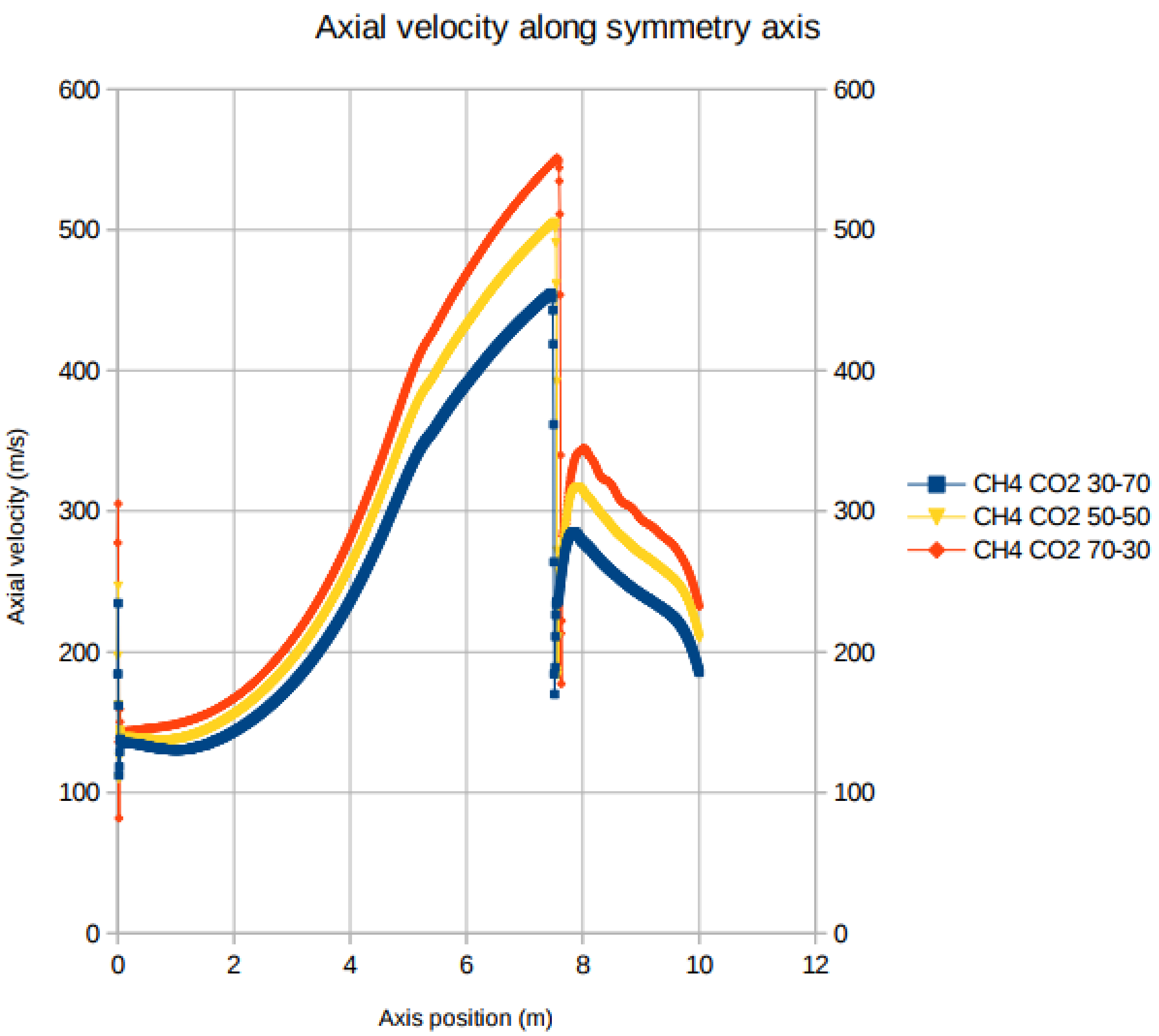

Figure 7. Comparison of axial velocity along the axis of the flow with mixture at different compositions

Observing the Figure 6, it is seen that there is a direct relation between the increase of CH_4 in the mixture composition and the increase of the velocity field of the flow. This can be associated with the decrease of the density of the mixture, because CH_4 has a lower molar mass than CO_2, and consequently there is a decrease of the necessary energy to accelerate the mixture. Therefore, as the available energy is kept constant the flow reach higher speeds.

6. PHASE SEPARATION SIMULATION

As the main objective of the research, was to verify the separation of two fluid phases, we carried out simulations using the boundary conditions indicated in Table 3 and the fluid was a mixture of liquid water and air.

Table 3. Boundary conditions for multiphase flow simulation.

Magnitudes	Inlet	Outlet
Total Pressure (Pa)	185000	-
Static Pressure (Pa)	-	83048
Static Temperature (K)	288	-
Rotation (rpm)	1500	-
V_{air}/V_{total}	0,999	-
V_{water}/V_{total}	0,001	-

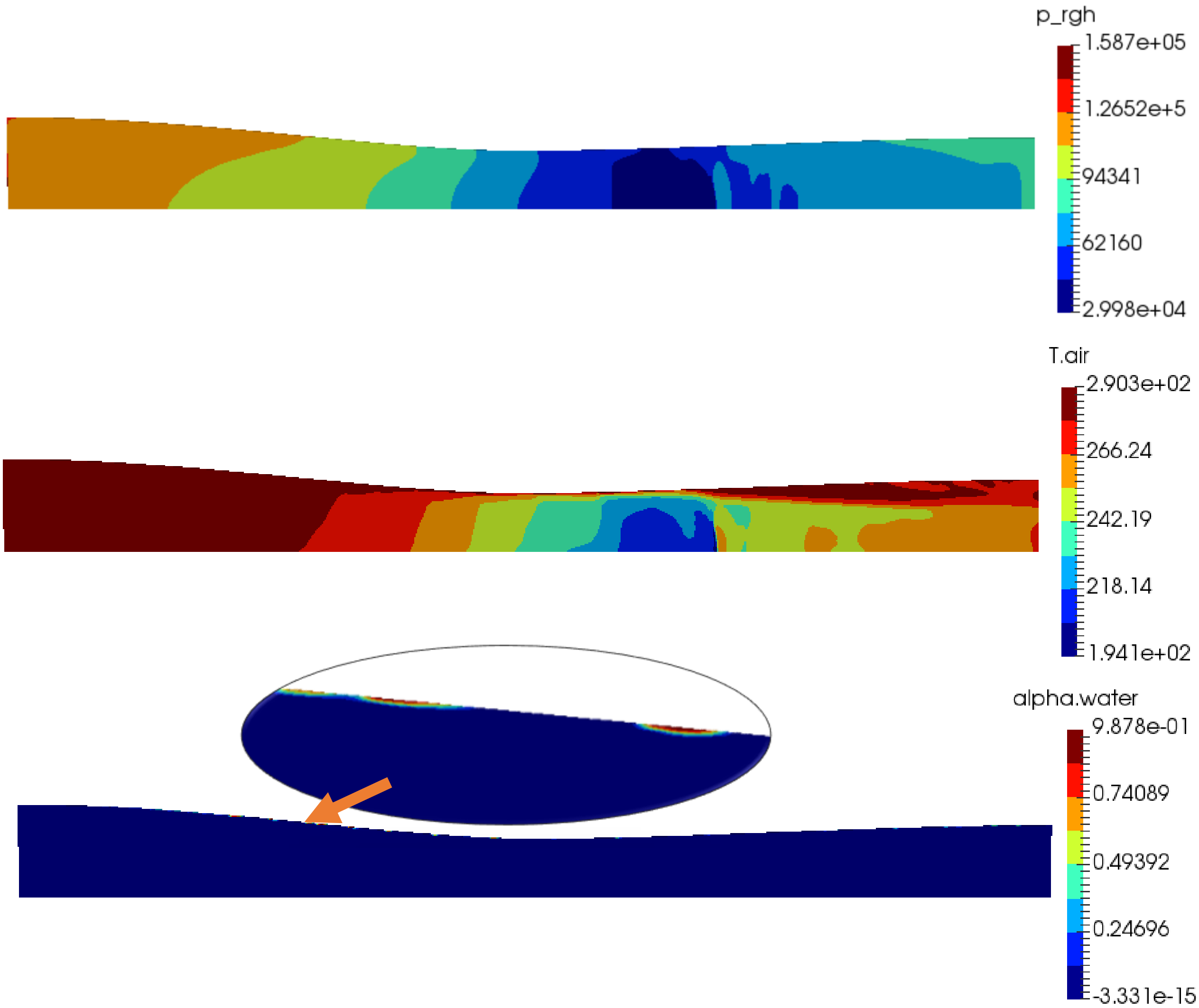

Figure 8. Static pressure and temperature and volume fraction of water fields of the multiphase simulation

As there is the presence of other fluid phase in the flow it is noticed that the flow is very affected by the interation of the two phases, as shown in Figure 7, which can be verified by comparing the behavior of the normal shock that occurs in the flow. Besides that, it is seen that the temperature and pressure fields are changed too almost exclusively in the normal shock and in the peripheral region.

7. CONCLUSIONS

As the simulations were carried out and the results were analyzed the main objective of the research of better understanding the flow behavior was achieved. It is possible to conclude that the presence of a secondary flow in the inlet generate the centrifugation of the denser fluid and the separation process occurs. It was also possible to investigate the application of different models in the numerical simulations for the flow prediction. The results shows that for the flow conditions that were tested the turbulent ideal gas model is a good model to make preliminary simulations as it is a relative accurate model and is computationally cheaper then more complex models.

8. ACKNOWLEDGEMENTS

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