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3D Unsteady RANS Computation of the Mixing on a T-junction

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Abstract

Turbulent mixing is a very common phenomenon in industrial processes. It is well know that the turbulence model has a massive impact on the accuracy of a turbulent flow, principally when it is used in processes of turbulent mixing. For this reason, this paper aims to investigate the impact of two specific turbulence models on calculating a mixture of gas-gas, using a 3D T- junction geometry. The differences between the calculation with two RANS based model, the kw-SST and SAS are investigated here. A mixture of Air and N_2 is performed. The sensibility of the refinement of the mesh of calculation is assessed to calculate the discretization error. A comparison of results obtained with the distinct models of turbulence is made with available experimental data. In this comparison it is showed that the SAS model, due to its capability of capturing some vortexes that SST couldn't, offers a better accuracy, with an error maximum bellow the 7%, in comparison to the experimental data.

Keywords: T-juntion, Turbulent mixing, RANS, CFD

1. Introduction

The mixing processes are very used in the industry. Typically, the mixing corresponds to the manipulation of a heterogeneous physical system in order to achieve homogeneity. In many cases in the industry the mixing of components is due to turbulent phenomenon [1].

The turbulent mixing is common described by two distinguished mixing scales [2]. First is macro- mixing, that is characterized by the big scales of vortexes that essentially distribute the diverse particles in the domain of the flow. In this scale is the inertial effects that are important. Second is micro-mixing, where rates of molecular diffusivity of mass and momentum correlate with the time needed to diffuse the momentum into the target smallest turbulent flow eddies and, correspondingly, the mass into the target smallest concentration variation. Eventually the effects can be also targeted at the molecular scale. Between both mixing situations we can also define a meso-mixing, this is achieved by actuating typically on the turbulence. In this case the turbulent kinetic energy, at the feed point to the mixer, must be enough to blend the added gas with the existing one [3].

One of the simplest geometries to study only the turbulent mixing is by crossing two flow streams. This can be done with a T-junction [4]. The T-junction results allow an assessment on the accuracy of the numerical simulations, this is useful to predict the accuracy of more complex geometries, for example mixing chambers.

The complexity of the turbulent mixing phenomena can be computational calculated applying directly the unsteady Navier-Stokes equations. The direct application of this equations is known as Direct Numerical Simulation (DNS). However, this approach needs very fine mesh and that leads to a computational cost very high and not effective for complex geometries present in the industry. Therefore, have been developed models of turbulence based in the Reynolds average equations for the Navier-Stokes equations. These models know as RANS resolve the mean proprieties of the flow and modulate the fluctuations [5].

In our investigations the use of models of turbulence based on the RANS equations are made to study the turbulent mixing of two gases in a T-junction. From a computational view point numerical simulation of two phases flow is complex and especially when is use a mixture of gases since the inertial effects are low and the molecular diffusion are slow [6].

2. Numerical Models for Turbulent Mixture with Multispecies

Since we are dealing with multispecies the Euler-Euler approach will be used by resorting to the ANSYS FLUENT commercial solver. As the objective is to compute the mixing of two gases the MIXTURE model was selected. This model is adequate to compute flows in which inertial forces are of relatively lower importance, since we are modelling gases. In this case all the species will be considered as a continuum and, for each one, mass, momentum and energy conservation equations will be applied. The variables for each specie will be afterwards coupled using weighted coefficients. Furthermore, the model solves the continuity, moment and energy conservation [7].

For this investigation was chosen the model $k-\omega\ SST$ in an unsteady mode (URANS). This model was chosen because as the aggregation of the qualities of the $k-\varepsilon$ standard for regions far away from the wall and the qualities of the $k-\omega$ for regions close to the wall [8]. This is possible due to the integration of the cross diffusion and the blending function. The $k-\omega\ SST$ resolves two transport equations, one for the turbulent kinetic energy, k, and other to the specific turbulence dissipation rate, ω [9].

Due to the importance of the small scales to the effectively mixture was investigated the capability of the SAS turbulence model. The SAS model is an upgrade of the $k-\omega\ SST$ that insert a source term, Q_{SAS}, in the ω transport equation. This term source is correlated to the von Kármán length scale making the model “scale-adaptive” [10].

A pressure-based solver was used with the coupled approach. A second order spatial discretization was defined altogether with the PRESTO! scheme, since this is a robust option for multiple species flows.

The models above described were used with the default configurations of the ANSYS FLUENT software [7].

3. Geometry and Methodology of the Test Case

A simple T-junction is composed by a main cylindrical duct that is perpendicular intersected by another. The test case geometry is composed by a main duct with a diameter D = 0.1 $[m]$ and a length of L = 0.5 $[m]$. The main duct is perpendicular intersected by a secondary cylindrical duct. The secondary duct has a diameter d = 0.026 $[m]$. At the inlet of the main duct the flow is AIR and is composed by 79% of N_2 and 21% of O_2. In the secondary duct is injected a pure flow of N_2.

The rate between each inlet is the mixing rate, defined in terms of the volumetric flowrate. This T-junction setup was experimental tested [11] and the results used to comparation. The experimental tests were conducted for a Reynolds number of 10 000. The mixing of air and N_2 has a kinematic viscosity of $\upsilon = 1.1504{\cdot}10^{-5}$ [Pa s], with the inlet velocity obtained from the Reynolds number.

The numerical simulations have been performed for two different mixing rates, defined by the fowling expression:

$$\frac{Q_{N_2}}{Q_{Ar}} = \frac{u_{N_2}}{u_{Ar}} \cdot \left(\frac{d}{D}\right)^2 \tag{1}$$

Here u is the velocity magnitude at the corresponding inlet. The velocity at the inlet of Ar was kept constant at 1.510 [m/s]. The inlet velocity of the secondary duct is 2.157 [m/s] and 4.314 [m/s] for the mixing ratios of 0.1 and 0.2, respectively.

For the model SST was made a sensibility test of the mesh to assessment if the mesh is enough accurate. For this propose we use the Mesh Convergence Index (GCI) [12] for that was discretized three unstructured meshes in a mesh generator. The sensibility of the mesh was made for a mixing ratio of 0.2.

After was use the model SAS in the finest mesh to assessment the resolution of the vortices. All the meshes have an integration of the mesh in to the wall. So, the surfaces mesh was inflated with a specific initial height so that the conditions of the nondimensional distance to the wall of the first node, y+, were close to the unit. Furthermore, the grow rate in the inflated cells was set to 1.2 for 10 cells for a good resolution of the effects of the wall in the flow.

The time step was always kept as 1[ms] since the maximum velocity in the system is 4.314 [m/s] and the characteristic length of the finest mesh can be approximated as 5 [mm]. Through the simulations the average velocity and the volume fraction, at the outlet, were monetarised. With these monitors was considerate that a full-time flow of 2 seconds gives enough time for the flow stabilization (time convergence).

4. Results and Discussion

The validation of the resolution of the wall was made since the y^+ of the first cell to the wall, is always, for all the simulations, bellow 4.

The assessment of the sensibility of the mesh of calculations was made by generating three mesh and use the Mesh Convergence Index (GCI), according to [12]. The coarse (Mesh 1), medium (Mesh 2) and fine (Mesh 3) have a total number of nodes to calculation equal to 29 671, 56 000 and 112 912, respectively. The mesh was generated in a way that the increase of refinement is bigger than 1.3. For calculate the increase of refinement was set a representative mesh length, h, calculated with the fowling expression:

$$h = \left[\frac{1}{N}\sum_{i=1}^{N}(\Delta V_i)\right]^{\frac{1}{3}} = [V med]^{\frac{1}{3}} \tag{2}$$

The sensibility of the mesh was study through the analyse of the two most critical variables that we want to study. The two critical variables are the *Volume Fraction of* N_2 and the *Pressure*.

The graphics represented in the Figure 1 show that the volume fraction of N_2 is more susceptive to the mesh refinement, specifically in the most critical region of mixing and turbulence that is the region ahead of the injection of the secondary flow.

The calculation of the GCI has made with a safety factor, Fs, equal to 1.5, since the mesh are unstructured. The results can be seen on the Table 1. The *GCI fine* is the error of the discretization of the finest mesh calculated and shows an error below 5%. This low error means that the values obtain in the inlet and outlet are little sensible to the mesh refinement.

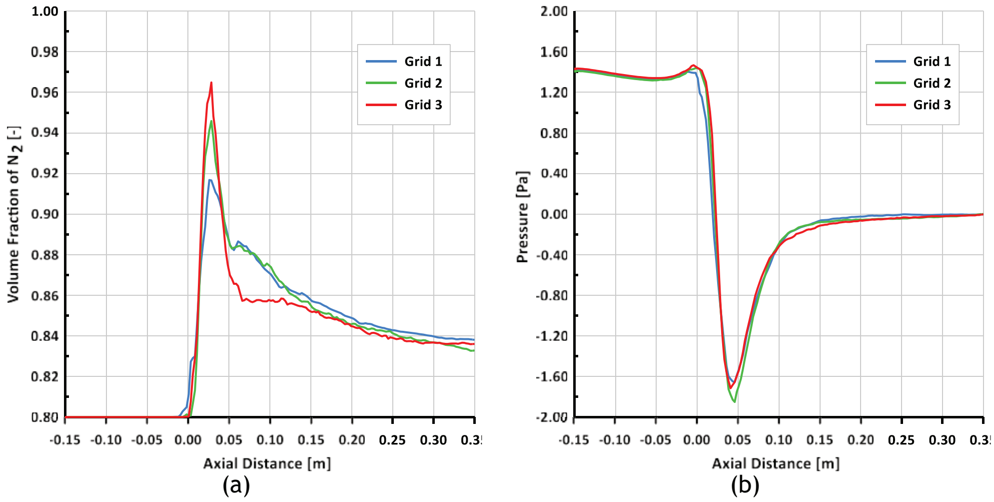

Figure 1: Variation of (a) Volume fraction of N_2 and (b) Pressure along the axis of the main duct. Note: At 0 [m] is where the axis of the secondary duct signs.

TABLE 1: Calculations for the discretization error based on the Mesh Convergence Index (GCI). Note: PhiX is the value of the variable correspond to the column to the MeshX.

	Pressure Loss	Volume Fraction N_2 (Outlet)
Vmed [m^3]	8.700e-8; 3.661e-8; 1.665e-8	
h [m]	4.443e-3; 3.321e-3; 2.554e-3	
Phi1	1.472 [Pa]	8.299e-1 [-]
Phi2	1.482 [Pa]	8.300e-1 [-]
Phi3	1.501 [Pa]	8.304e-1 [-]
r21	1.300	
r32	1.334	
GCI fine	1.264 %	0.0430 %
Phi-exact	1.513 [Pa]	0.831 [-]

Using the fine mesh was performed the calculation using the SAS model. We can see, in Table 2, that both turbulence models provide results with good accuracy. The SST model for mixing ratios of 0.1 and 0.2 presents a relative difference of 2.11% and 12.77%. The SAS model presents a much better result with a relative difference of only 1,13% e de 6,70%, respectively.

TABLE 2: Results comparison against experimental data [11] of the mean deviation of the mass fraction of N_2 at the outlet.

Q_{N_2}/Q_{Ar}	Experimental	SST	SAS
0.1	0.0205	0.0200	0.0208
0.2	0.0131	0.0148	0.0123

A view of the stream traces calculated from the secondary inlet are showed in Figure 2. It shows that the SAS model compute with more detail the turbulent structures created after the N_2 injection point, in that region the SST presents almost a linear flow distribution. Due to this difference the distribution volume fraction of N_2 is visibly affected.

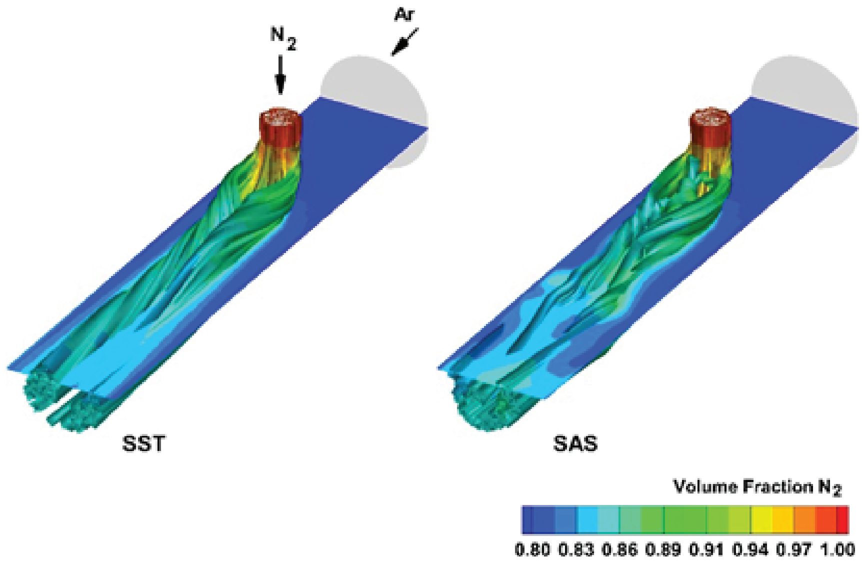

Figure 2: Stream traces calculated from the inlet of N_2 and a contour slide across the axial direction of the main duct, for the SST and SAS model. The contour presents the volume fraction of N_2.

The reason for this must relies in the vortex's formation. To analyse the vortexes structures we resort to the Q-criteria. The Q_{cr} relates the shear stress with vorticity magnitude locally in the flow. For values of Q_{cr}>0 we can see areas where the vorticity is bigger that shear stresses, also entailing a higher pressure than the other surroundings. This is given by the expression (3).

$$Q_{cr} = \frac{1}{2}(\|\Omega\|^2 - \|S\|^2) \tag{3}$$

Defining Ω as the vorticity tensor and S the deformation rate tensor. Choosing the appropriate value and calculating the iso-surface we can see the structures.

The value of 1000 [s^{-2}] was selected and can be seen in the Figure 3. In this figure is clear that the SAS model generated more vortexes structures after the region of injection of the secondary flow.

5. Conclusions

The GCI index as showed that, for the conditions tested, the mesh used is refined enough. Was possible to visualise the importance of the small vortexes in the diffusion

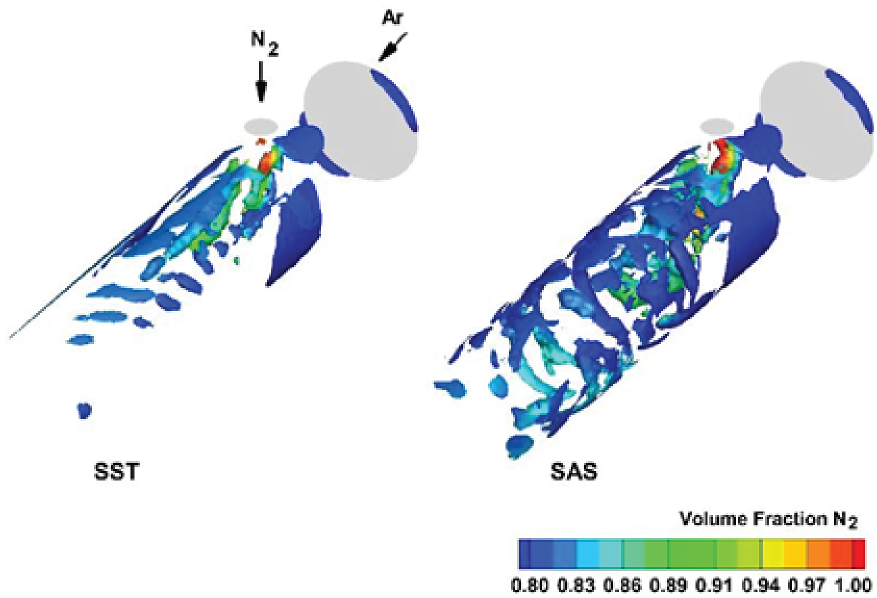

Figure 3: Q criterion with a value of 1000 [s-2] colorized by the volume fraction of N_2 for the calculation with the SST and SAS model.

of the species and provide a better mixture. In this way the SAS model with is active adaption to the length scale provide good results in the computation of the macro and meso mixing of gas-gas flow. A comparison with available experimental data showed that the SAS model as given a better result, a maximum error of 7%, compared to the SST results that as given a maximum 13% of error.

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