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"Utilização do método da PDF transportada para a avaliação de mistura entre componentes químicos"

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Use of the transported PDF method for evaluating mixtures between chemical components.

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Introduction

The probability density function (PDF) method has been used since 1969, when Ludgreen derived, modeled, and solved the transport equation for the joint velocity PDF. Subsequently, between 1974 and 1976, Dopazo, O'Brien, and Pope derived, modeled, and solved the transport equation for the joint composition PDF. This method is based on the analysis of certain points in the flow at each instant, using statistics to estimate it. In the present work, this was done through the study of Lagrangian particles.

According to Vedovoto[1], there are two methods for finding density functions, the first is to assume that the density function has a particular shape parameterized by the initial momenta. However, this is a rather imprecise method when complex chemical effects are taken into account. Another more efficient method is to obtain the joint PDF directly from its transport equations, a method called the joint compositional PDF method.
In this study, the second method was chosen to allow for the subsequent application of more chemical effects.

The closure model proposed by Villermaux and Deville[6], known as IEM (interaction by exchange with the mean) or LMSE (linear mean-square estimation), was chosen for modeling scalar transport in the composition space. In cases of molecular mixtures, this model is based on the reduction of scalar fluctuations, which refers to the instantaneous tendency of scalars towards their local mean.

Furthermore, the Cantera software[5] was used to provide the most accurate thermodynamic properties for each chemical species to complement chemical kinetics in future work.

Modeling

A cube of dimension 1 m³ is proposed as the control volume , through which **Hÿ** enters from the left and **Oÿ** from the right with constant velocities VÿHÿ and VÿHÿ , respectively. Thus, at each instant of time, the particle's position is updated by equation 1.

$$Xÿ\ n = Xÿ\ nÿ1 + Vÿ \times ÿt \quad (1)$$

To analyze the composition of each particle, the variable ÿ was created and defined from equation 2, such that Xi is the mass fraction of the element, i.e., Ns is the number of species.

$$ÿ = \{X1, X2, ..., XNs\} \quad (2)$$

Using the IEM-LMSE closure model, we arrive at equation 3, which, when discretized, can be written as as per equation 4. Given that ÿÿ is the chemical reaction rate, which is zero, since this work is only analyzing the micromixture, and ÿm is the mixing frequency defined in equation 5, where **Cÿ** is a constant, ÿ is the coefficient of diffusion, ÿt is the turbulent diffusion coefficient and ÿG is the filter size.

$$\frac{d\ddot{y}}{dt} = \ddot{y}\ddot{y}m(\ddot{y}\ \ddot{y}\ \bar{\ddot{y}}) + \ddot{y}\ddot{y} \tag{3}$$

$$\ddot{y}n = \ddot{y}n\ddot{y}1 + (\ddot{y}\ddot{y}m(\ddot{y}n\ddot{y}1\ \ddot{y}\ \bar{\ddot{y}}n\ddot{y}1) + \ddot{y}\ddot{y}) \times \ddot{y}t \tag{4}$$

$$\ddot{y}m = \ddot{y}2\ \frac{C\ddot{y}(\ddot{y} + \ddot{y}t)}{G} \tag{5}$$

For this simulation, **Cÿ** was used as 2, the value generally used according to Haworth. [3], the values of ÿ and ÿt used were based on equation 6, where ÿ is the kinematic viscosity and Sc is the number of Schmidt, while the time step, velocity, and ÿG were defined empirically.

$$\ddot{y} = \ddot{y}/Sc \tag{6}$$

From equation 4, the initial conditions, and the simulation parameters specified in Table 1, it is possible Develop a computer program as shown in Figure 1.

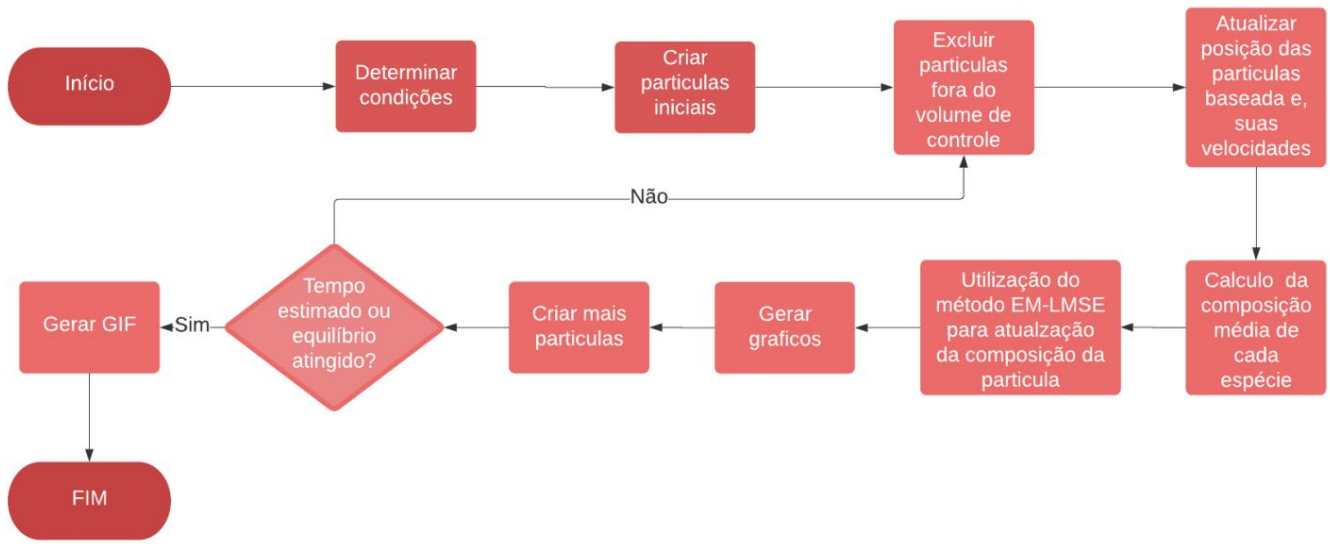

Figure 1: Flowchart

Parameter	Value
ÿt	0.1 s
VÿH2	(0, 0, 0.01) m/s
VÿO2	(0, 0, ÿ0.01)m/s
Cÿ	2
ÿG ÿ	0.1
ÿt	0.001
	0.001

Table 1: Parameters

Results and Conclusions

It is possible to visualize the control volume as a function of **H2** composition in Figures 2, 3 , and 4 at the following times. t=0 s, t=25 s, and t=50 s, respectively. However, for a quantitative analysis, the distribution of composition over time (PDF) in figures 5, 6 and 7 at times t=0 s, t=25 s and t=50 s, respectively. Therefore,

It can be seen that, as expected, the average composition of both **O2** and **H2** changes over time.

They tend towards the average.

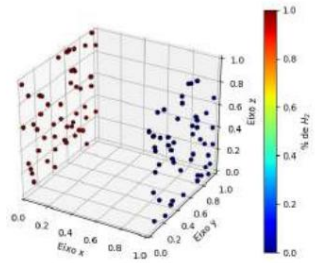

Figure 2: 3D visualization at t=0 s

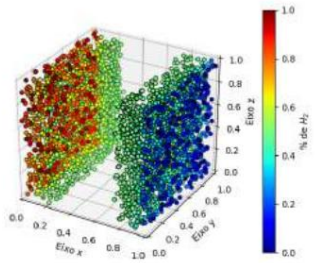

Figure 3: 3D visualization in t=25 s

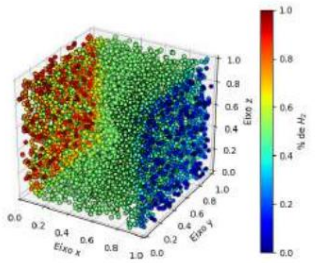

Figure 4: 3D visualization in t=50 s

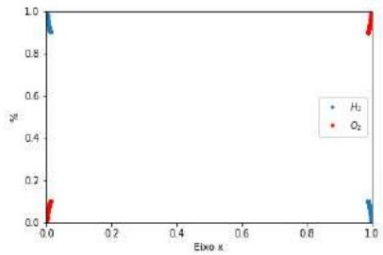

Figure 5: Composition at t=0 s

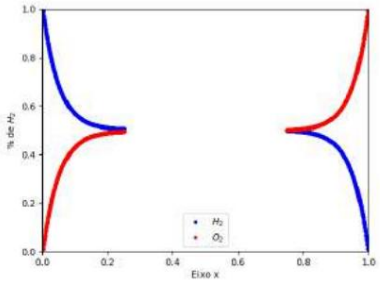

Figure 6: Composition at t=25 s

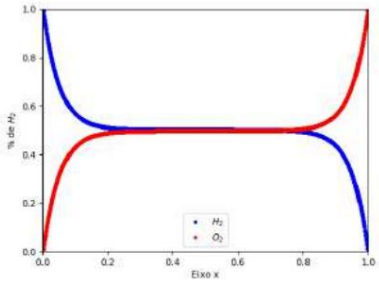

Figure 7: Composition at t=50 s

Finally, it is possible to analyze the cumulative distribution function in figures 8, 9 , and 10 , and the real density function of... problem in figures 11, 12 and 13.

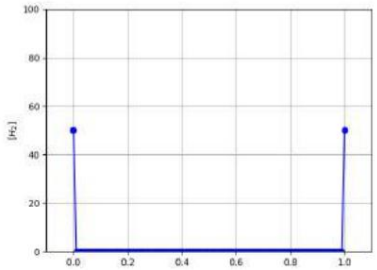

Figure 8: CDF function at t=0 s

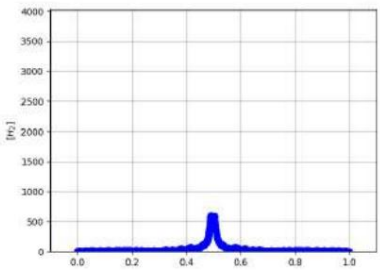

Figure 9: CDF function at t=25 s

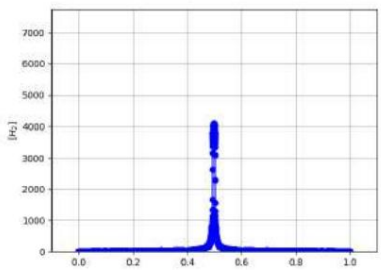

Figure 10: CDF function at t=50 s

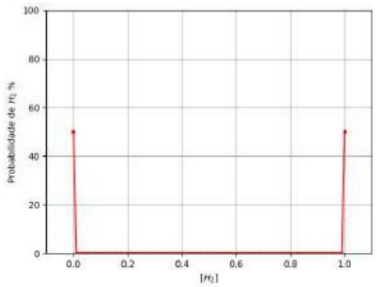

Figure 11: PDF function at t=0 s

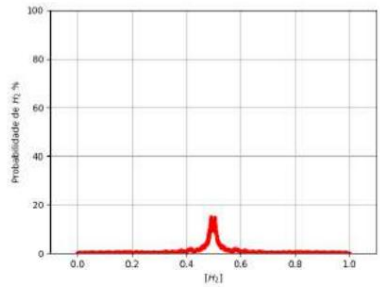

Figure 12: PDF function at t=25 s

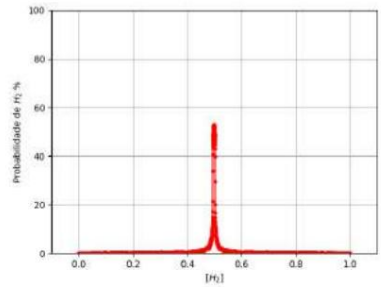

Figure 13: PDF function at t=50 s

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