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# Modeling and Simulation of Laminar Jet Diffusion Flames of Methyl Butanoate

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**Abstract**. The aim of this work is to obtain the mass fraction of the species involved in a two step mechanism for a biodiesel surrogate, methyl butanoate (MB). For this, the solution for the one-step and two-step models was used and the flow equations were solved. The equations were discretized by the finite difference method and were integrated by the Simplified Runge-Kutta method. The results obtained agree with data from the literature.

**Keywords**. Methyl butanoate, Jet diffusion flame, Burke-Schumann solution, CFD, Simplified Runge-Kutta method.

## 1 Introduction

Biofuels are solid, liquid or gaseous fuels that are produced from starch, sugar, oil and raw materials obtained through the cultivation of wheat, corn, sugar cane, among others [13]. Biofuels are produced from biomass and waste materials from the food industry, forestry, etc. They include: bioethanol derived from lignocellulose, biodiesel obtained by refining used vegetable oils, etc.

Biodiesel can be reasonably represented by simpler surrogate fuels that are of the same ester class [3, 7]. For example, MB ($C_5H_{10}O_2$) contains the essential chemical structure of large chain fatty acids, and is a reasonable surrogate for flames of biodiesel at high temperatures.

Models of reactive flowns using Computational Fluid Dynamics (CFD) equations are complex [10]. The mathematical formulation of CFD consists of coupled nonlinear partial differential equations such as: continuity, momentum and mixture fraction, which can be discretized using, e.g., methods as finite differences and finite elements [6, 8].

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The aim of this work is to model the mass fraction of the biofuel surrogate, MB, for one and two-step mechanism and solve the flow equations. The solution of these equations is approximated by the Simplified Runge-Kutta method.

# 2 Model formulation

## 2.1 Burke-Schumann solution

Diffusion flames can be described by the conservative scalar $Z$, which represents the mixture fraction. The mass fraction of the unburned fuel is $Y_{F,u} = Y_{F,1}Z$, where $Y_{F,1}$ is the mass fraction of the fuel in the initial stream. Since $(1 - Z)$ represents the mass fraction of the oxidant, we can also write $Y_{O2,u} = Y_{O2,2}(1 - Z)$, where $Y_{O2,u}$ is the mass fraction of the unburnt oxidant and $Y_{O2,2}$ is its mass fraction.

Considering the global one-step reaction [11, 12]

$$\nu_F[F] \; + \; \nu_{O_2}[O_2] \; \rightleftharpoons \; \nu_{CO_2}[CO_2] \; + \; \nu_{H_2O}[H_2O], \tag{1}$$

where $\nu_i$ is the stoichiometric coefficient of the species $i$, we have that the relation between the mass fractions of the fuel and the oxidant is given by $\dfrac{dY_{i_1}}{\nu_{i_1}W_{i_1}} = \dfrac{dY_{i_2}}{\nu_{i_2}W_{i_2}}$, where $W_i$ represents the molecular weight of the species $i$.

Integrating the last equation, with the subscripts $i_1 = F$ and $i_2 = O_2$, between the initial unburnt state and another posterior state, we have $\frac{Y_F - Y_{F,u}}{\nu_F W_F} = \frac{Y_{O_2} - Y_{O_2,u}}{\nu_{O_2} W_{O_2}}$. Then

$$\nu Y_F - Y_{O_2} = \nu Y_{F,u} - Y_{O_2,u}, \tag{2}$$

where $\nu = \frac{\nu_{O_2} W_{O_2}}{\nu_F W_F}$ is the stoichiometric ratio.

From equation (2), we write the mixture fraction $Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}}$. For a stoichiometric mixture, $\nu Y_F = Y_{O_2}$. Then the stoichiometric mixture fraction is given by $Z_{st} = \left(1 - \nu \frac{Y_{F,1}}{Y_{O_2,2}}\right)^{-1}$.

The solution of the global one-step mechanism can be approximated by the Burke-Schumann solution, which describes the mass fraction of the species involved in the reaction with respect to the mixture fraction Z [2]. For $Z \leq Z_{st}$, combustion ends when all fuel is consumed and the misture fraction result in:

$$\begin{cases} Y_{F,b} = 0; \\ Y_{O_2,b} = Y_{O_2,u}\left(1 - \dfrac{Z}{Z_{st}}\right); \\ Y_{CO_2,b} = Y_{CO_2,st}\dfrac{Z}{Z_{st}}; \\ Y_{H_2O,b} = Y_{H_2O,st}\dfrac{Z}{Z_{st}}. \end{cases} \tag{3}$$

For $Z > Z_{st}$, the combustion is complete when all oxygen is consumed and the equations result in:

 

$$\begin{cases} Y_{F,b} = Y_{F,1}\left(\dfrac{Z - Z_{st}}{1 - Z_{st}}\right); \\ Y_{O_2,b} = 0; \\ Y_{CO_2,b} = Y_{CO_2,st}\left(\dfrac{1 - Z}{1 - Z_{st}}\right); \\ Y_{H_2O,b} = Y_{H_2O,st}\left(\dfrac{1 - Z}{1 - Z_{st}}\right); \end{cases} \tag{4}$$

where $Y_{CO_2,st} = \dfrac{\nu_{CO_2} W_{CO_2}}{\nu_F W_F} Y_{F,1} Z_{st}$ and $Y_{H_2O,st} = \dfrac{\nu_{H_2O} W_{H_2O}}{\nu_F W_F} Y_{F,1} Z_{st}$.

In a mechanism of more than one step, we write the mixture fraction in the form: $Z = Z_1 + Z_2 + \cdots + Z_n$, where $n$ are the components. In terms of the mass fraction of the species [1], we have:

$$Z_1 = \frac{Y_F}{Y_{F,1}};\ Z_k = \frac{\nu_F W_F}{\nu_k W_k}\frac{Y_k}{Y_{F,1}};\ k = 2, \cdots, n; \tag{5}$$

so that when we replace (5) in the mass fraction equation of the species

$$\rho\frac{\partial Y_k}{\partial t} + \rho\vec{u}\cdot\vec{\nabla}Y_k = \vec{\nabla}\cdot(\rho D\vec{\nabla}Y_k) \pm \dot{\omega_k}\ ;\ k = 1, \cdots, n; \tag{6}$$

we obtain

$$\rho\frac{\partial Z_k}{\partial t} + \rho\vec{u}\cdot\vec{\nabla}Z_k = \vec{\nabla}\cdot(\rho D\vec{\nabla}Z_k) \pm \dot{\omega_k}\ ;\ k = 1, \cdots, n. \tag{7}$$

Adding the $n$ equations in (7) gives the equation of the mixture fraction described in (8). The solution of the set of $n$ equations is obtained numerically.

## 2.2 Flow equations

In order to formulate the system of equations that model the flow of a free jet, we consider the following hypotheses: i) the flow is two-dimensional and laminar; ii) the flow regime is permanent and the fluid is incompressible; iii) field forces are negligible.

The flow will be described by the dimensionless equations of continuity, momentum, pressure and mixture fraction [5]:

$$\begin{cases} \nabla\cdot\vec{u} = 0; \\ \dfrac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\vec{\nabla}\vec{u} = -\dfrac{1}{\rho}\vec{\nabla}p + \dfrac{1}{Re}\nabla^2\vec{u}; \\ \nabla^2 p = 2\left(\dfrac{\partial u}{\partial x}\dfrac{\partial v}{\partial y} - \dfrac{\partial u}{\partial y}\dfrac{\partial v}{\partial x}\right); \\ \dfrac{\partial Z}{\partial t} + \vec{u}\cdot\vec{\nabla}Z = \dfrac{1}{ReSc}\nabla^2 Z; \end{cases} \tag{8}$$

where $Re = \frac{uL}{\nu}$ is the Reynolds number, which determines the fluid flow regime, $Sc = \frac{\nu}{D}$ is the Schmidt number, which relates the viscosity and the mass diffusivity of the fluid.

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Considering the domain $\Omega = \{(x, y) : \ 0 \leq x \leq 1 \ , \ 0 \leq y \leq 0.1\}$, the initial and boundary conditions are given by:

$$\begin{cases} \vec{u} = (u, v) = (1, 0), \ p = Z = 1, \ \text{for } t = 0, \ \forall\Omega; \\ u = Z = \begin{cases} 1, \ \text{if } 0.045 \leq x \leq 0.055 \\ 0, \ \text{otherwise} \end{cases}, v = \frac{\partial p}{\partial x} = 0, \ \text{for } (0, y) \in \Omega; \\ u = v = Z = \frac{\partial p}{\partial x} = 0, \ \text{for } (x, 0) \in \Omega; \\ u = v = Z = \frac{\partial p}{\partial y} = 0, \ \text{for } (x, 0.1) \in \Omega; \\ \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial Z}{\partial x} = 0, p = 1, \ \text{for } (1, y) \in \Omega. \end{cases} \tag{9}$$

### 2.3 Numerical formulation

The Simplified Runge-Kutta method [1] is used because of the small number of operations required. The coefficients of the method were chosen to obtain a solution with high temporal precision. For the system of differential equations $\frac{\partial \vec{W}}{\partial t} = -\vec{R}$, the Simplified Runge-Kutta method is:

$$\begin{cases} \vec{W}_{(i,j)}^{(0)} = \vec{W}_{(i,j)}^{(n)}; \\ \vec{W}_{(i,j)}^{(k)} = \vec{W}_{(i,j)}^{(0)} - \alpha_r \Delta t \vec{R}_{(i,j)}^{(k-1)}; \\ \vec{W}_{(i,j)}^{(n+1)} = \vec{W}_{(i,j)}^{(k)}; \end{cases} \tag{10}$$

where $\vec{R}$ is the vector representing the system of equations evaluated at points $(i, j)$ of the domain, in stage $k$, $k = 1, \ldots, n$; $\vec{W}$ contains the variables of interest of the problem; $\Delta t$ is the time step and $\alpha_r$ are the coefficients of the method. For second order temporal approximation with 3 stages, we take $\alpha_1 = \alpha_2 = 0.5$ and $\alpha_3 = 1$.

## 3 Numerical results

The equations of the flow were discretized using the finite difference method, in which one replaces the derivates of the differential equations by approximations involving only numerical values [4,14]. Consider a jet as shown in Figure 1, in the domain $\Omega$, whose nozzle diameter is $d \simeq 0.01$. A non-uniform mesh was used, refined on $\Omega$ at the beginning and centerline of the jet, with 151x51 points. The dimensionless numbers taken were $Re = 2400$ and $Sc = 0.5$. The Simplified Runge-Kutta method was applied using $\Delta t = 10^{-6}$, from which numerical data for the laminar diffusion flame mixture fraction were obtained.

Figure 1 shows the isolines of mixture fraction for a laminar jet diffusion flame of MB.

A numerical result of mass fractions for MB diffusion flame can be obtained from the global two-step mechanism:

$$[C_5H_{10}O_2] + 4[O_2] \rightleftharpoons 5[CO] + 5[H_2O]; \tag{11}$$

$$[CO] + \frac{1}{2}[O_2] \rightleftharpoons 5[CO_2]. \tag{12}$$

Figure 2 shows the mass fraction as a function of the mixture fraction of the species of the laminar jet diffusion flame in the centerline of the jet. The maximum values for the

 

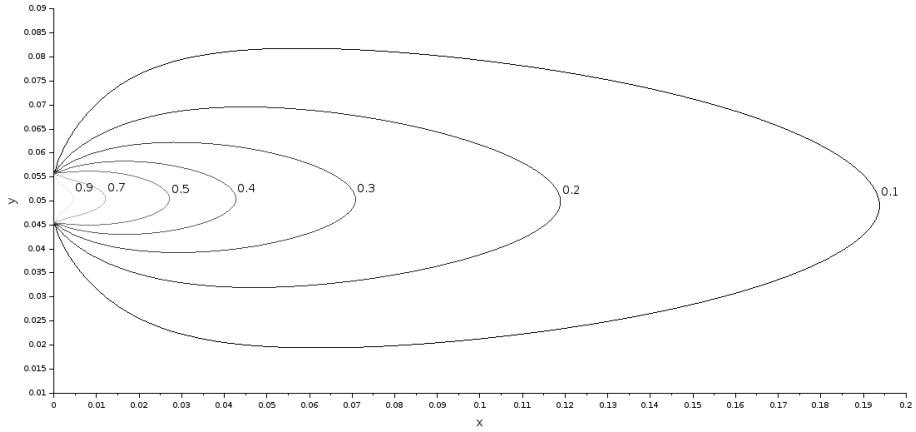


Figure 1: Isolines of the mixture fraction for diffusion flame of MB.

$H_2O$, $CO_2$ and CO species in the stoichiometric mixture fraction ($Z_{st} \cong 0.1025$) are the ideal conditions for burning.

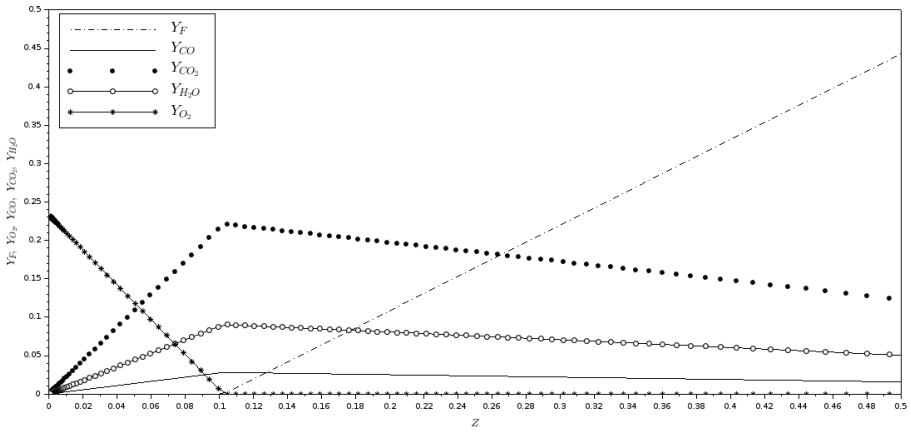


Figure 2: Mass fraction of the species along the centerline of the jet along Z.

The truncation error of the mixture fraction equation, for infinity norm is given by:

$$e_{\infty}^{N} = \max_{i=1,\ldots,N_p} |e_i^N|, \tag{13}$$

where $e_i^N$ is the mixture fraction difference in the iteration $N$ and $N-1$, for N = 2,3,.., and $N_p$ is the number of points of the mesh. The results shown in Table 1 indicate the

 

increase in accuracy of the Simplified Runge-Kutta method for the mixture fraction in the infinite norm.

Table 1: Error for mixture fraction equation.

| Iteration Error | Error ($E_\infty$) |
|---|---|
| 500000 | 1.8139601358664603E-007 |
| 1000000 | 3.5497390957206498E-008 |
| 1500000 | 2.8048385565526690E-008 |
| 2000000 | 1.6826276684478447E-008 |
| 2500000 | 9.1952749303736425E-009 |
| 3000000 | 4.8239832250301928E-009 |
| 4000000 | 1.2876340206753600E-009 |
| 5000000 | 3.6559603998689849E-010 |
| 6000000 | 1.1934498354848611E-010 |

## 4 Conclusion

In this work, we model a jet diffusion flame of methyl butanoate using a two-step mechanism to determine the mass fraction of the species with respect to the mixture fraction, given through the flow equations. The Burke-Schumann solution is used for the solution of the one step model. The numerical solution of the two step model and flow equations was obtained using the Simplified Runge-Kutta method and the convergence is shown in Table 1.

According to [9, 15], the results obtained for the mass fractions of MB, $O_2$, $CO$, $CO_2$ and $H_2O$ are coherent.

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