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 flows 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].
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]

$$
\nu_F[F] + \nu_{O2}[O_2] \rightleftharpoons \nu_{CO2}[CO_2] + \nu_{H2O}[H_2O],
$$

(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

$$
dY_i \nu_i W_i = dY_j \nu_j W_j,
$$

(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

$$
\nu Y_F - Y_{O2} = \nu Y_{F,u} - Y_{O2,u},
$$

(3)

where $\nu = \frac{\nu_{O2} W_{O2}}{\nu_F W_F}$ is the stoichiometric ratio.

From equation (2), we write the mixture fraction $Z = \frac{\nu Y_F - Y_{O2} + Y_{O2,2}}{\nu Y_{F,1} + Y_{O2,2}}$. For a stoichiometric mixture, $\nu Y_F = Y_{O2}$. Then the stoichiometric mixture fraction is given by

$$
Z_{st} = \left(1 - \frac{Y_{F,1}}{Y_{O2,2}}\right)^{-1}.
$$

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 mixture fraction result in:

$$
\begin{align*}
Y_{F,b} &= 0; \\
Y_{O2,b} &= Y_{O2,u}\left(1 - \frac{Z}{Z_{st}}\right); \\
Y_{CO2,b} &= Y_{CO2,2}\frac{Z}{Z_{st}}; \\
Y_{H2O,b} &= Y_{H2O,2}\frac{Z}{Z_{st}}.
\end{align*}
$$

(3)

For $Z > Z_{st}$, the combustion is complete when all oxygen is consumed and the equations result in:
where $Y_{CO_2,st} = \frac{\nu_{CO_2} W_{CO_2}}{\nu_F W_F} Y_F, 1 Z_{st}$ and $Y_{H_2O,st} = \frac{\nu_{H_2O} W_{H_2O}}{\nu_F W_F} Y_F, 1 Z_{st}$.

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:

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

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

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

we obtain

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

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]:

$$\begin{cases}
\nabla \cdot \bar{u} = 0; \\
\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \bar{\nabla} \bar{u} = -\frac{1}{\rho} \nabla p + \frac{1}{Re} \nabla^2 \bar{u}; \\
\nabla^2 p = 2 \left( \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \right); \\
\frac{\partial Z}{\partial t} + \bar{u} \cdot \bar{\nabla} Z = \frac{1}{Re Sc} \nabla^2 Z;
\end{cases}$$

where $Re = \frac{u L}{\nu}$ 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.
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:

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

(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:

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

(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 derivate 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 \( d \approx 0.01 \). 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:

\[
[C_5H_{10}O_2] + 4[O_2] \Rightarrow 5[CO] + 5[H_2O]; \quad (11)
\]

\[
[CO] + \frac{1}{2}[O_2] \Rightarrow 5[CO_2]. \quad (12)
\]

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$_2$O, CO$_2$ and CO species in the stoichiometric mixture fraction ($Z_{st} \approx 0.1025$) 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:

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

where $e_i^N$ is the mixture fraction difference in the iteration $N$ and $N - 1$, for $N = 2, 3, \ldots$, 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.

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<th>Iteration</th>
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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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References


