A Regenerative Multiple Flamelet Model for non-Premixed Combustion with non-Uniform EGR

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Abstract: - The conserved scalar approach is an attractive means to model turbulent combustion as it reduces the dimensionality of the reactive flow such that the reactive scalars are solved in a much more compact space. The present work extents the traditional flamelet approach in cases where the oxidizer stream has a non-uniform distribution of combustion products as exhaust gas recirculation (EGR) or residual gases. Finally the new approach, the so-called regenerative multiple flamelet (RMF) model, is compared with the RIF model using a simplified two dimensional CFD code.

Key-Words: - Flamelets, conserved scalars, reactive scalars, RIF model, RMF model, EGR, PPCI combustion.

1 Motivation

There are many combustion applications such as the diesel engine, in which fuel and oxidizer enter the combustion chamber in separate streams. In this case a very common approach to model turbulent combustion is by using the flamelet approach. For engine applications, the first attempt to use flamelet modeling in diesel combustion was done by Pitsch et al. [1] who proposed a methodology, namely the representative interactive flamelet (RIF) model, in which the reactive scalars are mapped into an unsteady laminar flamelet. Later, recognizing the limitation of the single flamelet approach in accurately representing the scalar dissipation rate distribution in the cylinder, Barth et al. [2] extended the RIF approach to multiple flamelets, where flamelets are created based on the history of the scalar dissipation rate. More recently, Hergart et al. [3] further improved the RIF approach to account for the wall heat transfer in the flamelet equations.

Although new technologies, i.e., fuel cells, have been proposed as an alternative to internal combustion engines, the partially premixed compression ignition (PPCI) engine has been considered an immediate solution to environmental and fuel economy concerns. Specifically, it seems to be a feasible practical solution to the many challenges in the homogeneous charge compression ignition (HCCI) engine development, by creating an overall lean, low-temperature combustion while providing a means to control the ignition timing simultaneously [4]. On the other hand, to model PPCI combustion is a new challenge as the current versions of the RIF model cannot be used in the PPCI combustion due to the non-uniform EGR content of the oxidizer stream.

To overcome this difficulty, the present work proposes an alternative mathematical formulation and modeling strategy that can adequately describe a turbulent non-premixed combustion with non-uniform EGR. The basic concept stems from the flamelet concept of utilizing conserved scalars, but the proposed model departs from the conventional flamelet model approach by utilizing two conserved scalars. The resulting laminar flamelet equations are similarly written as a function of the first variable, while the other variable provides a means to distinguish different flamelets based on the EGR composition of the oxidizer stream. Furthermore, the proposed model allows the flamelets to be mixed and reinitialized at every time in order to account for the history effects on the solution of the unsteady flamelets.

2 Model Formulation

2.1 A brief description of the RIF approach

In this subsection, the general concept of the flamelet approach, namely the RIF model [2], in diesel combustion is briefly reviewed.

In the RIF model a typical choice for the conserved scalar is the mixture fraction Z, defined as the elemental mass fraction. Accordingly, for unity Lewis numbers, the reactive scalars are described in the one-dimensional mixture fraction space by the following equation [5]:

$$\rho\frac{\partial\psi_i}{\partial t}=\rho\frac{\chi}{2}\frac{\partial^2\psi_i}{\partial Z^2}+\omega_i\ , \qquad (1)$$

where ψ_i is the i^{th} reactive scalar and ω_i the source term due to chemical reactions. An important parameter in the flamelet equations is the scalar dissipation rate defined as

$$\chi = 2D\left|\nabla Z\right|^2, \quad (2)$$

which represents the rate at which the reactive scalars are transported into the flame.

It is common in turbulent nonpremixed combustion to implement a presumed shape PDF approach to describe the statistics of the mixture fraction. In the RIF model the beta probability density function (β-PDF) is assumed [5], which can be defined uniquely by the first two moments of the mixture fraction, that is, the Favre mean , $\tilde{Z}$, and the Favre variance, $\widetilde{Z''^2}$. Then, from the knowledge of these two quantities at a given time and space, the Favre mean values of the reactive scalars can be computed in the physical domain.

For the implementation of the RIF approach the transport equations for $\tilde{Z}$, and $\widetilde{Z''^2}$ are solved by the CFD code along with the conservation equations for mass, momentum, and energy. Then, a separate unsteady flamelet equation solver is coupled to the CFD code which provides the solutions of the reactive scalars in the mixture fraction space and finally, the Favre mean value of the species mass fractions in the physical domain are computed by using the available statistics of the mixture fraction and the solution of the flamelet equations.

2.2 The conserved scalars

In the new approach an alternative definition of the mixture fraction is introduced based on the mass fraction of carbon in the reactive mixture, i.e.,

$$Z = \frac{\zeta_C}{\zeta_C^{FS}}, \quad (3)$$

where ζ_C , and ζ_C^{FS} are the carbon mass fractions of the gas mixture at a given location, and of the fuel spray, respectively. However, since knowledge of the mixture fraction is not sufficiently to determine the state of the reactive mixture due to the presence of the combustion products, an additional conserved scalar is introduced. Specifically, the initial EGR (combustion products) mass fraction is defined as the J variable

$$J = \frac{m_{\text{init\_EGR}}}{m_t}, \quad (4)$$

where $m_{\text{init\_EGR}}$ represents the mass of fluid originated by the initial exhaust gases (EGR) and m_t the total fluid mass at the specific location. Therefore, the J variable can take any value between zero (which represents pure air).

Then, using the above conserved scalars as the new independent variables, the fuel, the oxidizer and the combustion product streams can be represented by the following points $(1,0)$, $(0,0)$ and $(Z_{\text{EGR}},1)$, respectively in the (Z,J) plane as illustrated in Figure 1. Particularly, in the (Z,J) conserved scalar plane any mixture of fuel, oxidizer and combustion products (EGR or residual gases) must lie inside the triangular region that is defined by the aforementioned points [6], which is also presented in the figure.

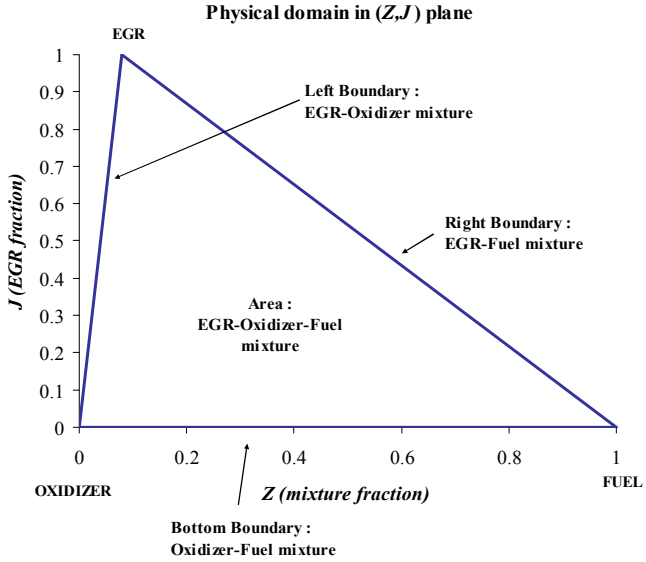

Fig.1, Representation of the physical domain (in the two dimensional conserved scalar plane) of any reactive system that consists of fuel, oxidizer (air) and combustion products (EGR).

2.3 Defining multiple flamelets in the conserved scalar plane.

It is important to take the following two factors under consideration in order to apply the conserved scalar approach in PPCI combustion. First, given that each flamelet represents a series of homogeneous reactors that interact with each other due to turbulence, the orientation of a flamelet in the (Z,J) conserved plane must align with the orientation of this interaction. In particular, in the PPCI combustion liquid fuel is injected into a non homogeneous mixture of air, combustion products and maybe some fuel from previous injection, which means that a flamelet should represent a counterflow flame of a fuel stream and an oxidizer stream with the above composition. Thus, based on the

inhomogeneity of the oxidizer stream, different flamelets can be created by assuming oxidizer streams with different composition. Therefore, the interaction due to turbulence occurs between the fuel and different oxidizer streams. Graphically, this can be interpreted that a flamelet should always represent a curve that connects the left boundary of triangle CFG in Figure 2 with the vertex F which corresponds to the fuel stream.

Second, from the definition of the J variable it is apparent that its minimum value must decrease during the evaporation of the fuel spray. Specifically, because the total mass at a specific location is increased due to the evaporated fuel, the value of the J variable has to be reduced respectively from mass conservation considerations. Therefore, defining the flamelets by representative values of the J variable is not appropriate since the minimum value of the J variable, $J_{\min}$, is decreasing due to EGR dilution by the evaporated fuel. Thus, knowing the $J_{\min}$ at time t is not enough to bound from below the J space at time $t+\Delta t$ and hence to accurately define the first flamelet which corresponds to mixtures with the smallest value of the J variable in the reacting flow.

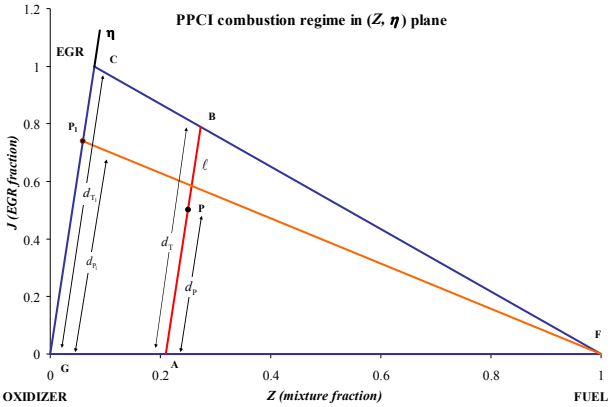

Fig.2, The η coordinate and the domain in the PPCI combustion.

From the above it is apparent that a new scalar needs to be introduced in order to define the flamelets in the (Z,J) plane. The new scalar is called the η variable and it is also a conserved scalar since it is a known function of the Z and J conserved scalars. Then, based on the η variable, the flamelet is defined as a counterflow flame between a fuel and an air-EGR stream. Besides, the η variable does not decrease by the increase of the total mass due to fuel evaporation. In order to calculate the η variable for an arbitrary point P, which is inside the physical domain as illustrated in Figure 2 and has coordinates $(Z_{\rm P},J_{\rm P})$, we calculate initially the slope of the line that passes from the specific point P and is parallel to the left boundary of the triangle CFG, as shown in Figure 2. This line, ℓ, intersects the bottom and the left sides of the triangle at the points A and B, respectively. Then, the value of the η variable at the specific point P is given by the ratio of the length of the segment AP normalized by the length of the segment AB, that is

$$\eta=\frac{d_{\rm p}}{d_{\rm T}}, \qquad (5)$$

where $d_{\rm p}$ represents the distance between points A and P, and $d_{\rm T}$ the distance between points A and B, which are given by the following formulas:

$$d_{\rm P}=\sqrt{\left(Z_{\rm P}-Z_{\rm A}\right)^2+\left(J_{\rm P}-J_{\rm A}\right)^2}, \qquad (6)$$

$$d_{\rm T}=\sqrt{\left(Z_{\rm B}-Z_{\rm A}\right)^2+\left(J_{\rm B}-J_{\rm A}\right)^2}, \qquad (7)$$

In the above equations, $(Z_{\rm A},J_{\rm A})$ and $(Z_{\rm B},J_{\rm B})$ are the coordinates of the points A and B, which are given by:

Point A: $(Z_{\rm A},J_{\rm A})=(-kZ_{\rm EGR},0)$, (8)

Point B: $(Z_{\rm B},J_{\rm B})=\left(Z_{\rm EGR}\left[1-k\left(1-Z_{\rm EGR}\right)\right],\frac{1-Z_{\rm B}}{1-Z_{\rm EGR}}\right)$, (9)

where k is the constant of the line ℓ that passes from point P and it is parallel to the left boundary of the triangle CFG, as illustrated in Figure 2. The line ℓ and its constant k are defined by the following equations

$$J=\frac{1}{Z_{\rm EGR}}Z+k, \quad (10) \qquad k=J_{\rm P}-\frac{1}{Z_{\rm EGR}}Z_{\rm P}, \quad (11)$$

The η variable, which takes values in the interval $[0,1]$, is a coordinate with orientation parallel to the left boundary of the physical domain, while its unit vector is compressed along the Z axis. A physical interpretation of the η variable is apparent if we assume that any mixture of oxidizer, fuel and EGR can be decomposed into two basic mixtures, one that consists of fuel and oxidizer and the other that consists of fuel and EGR. Then, these basic mixtures have the same fuel mass fraction as the original mixture, but the remaining mass fraction for the first basic mixture is due to the oxygen mass, and for the second basic mixture is due to the EGR mass. Based on the above decomposition, the η variable represents the mass fraction of the second basic

mixture, which is the corresponding fuel-EGR mixture of the original mixture, that is

$$\eta = \frac{m_{\text{F-EGR}}}{m_{\text{M}}}, \qquad (12)$$

where $m_{\text{F-EGR}}$ and m_{M} are the masses of the fuel-EGR and of the original mixture respectively. It should be mentioned that if the original mixture has no fuel, then the η variable coincides with the J variable.

Therefore, $\eta = 0$ corresponds to all mixtures which consist of any combination of fuel and oxidizer streams, and it represents the bottom boundary (segment FG in Figure 2) of the domain in the (Z,J) plane; while $\eta = 1$ corresponds to all mixtures, which consist of any combination of fuel and EGR streams, and it represents the right boundary (segment FC in Figure 2) of the domain in the (Z,J) plane. It is apparent that both lines, the $\eta = 0$ and the $\eta = 1$ define two different flamelets. The first corresponds to a flamelet that is formed from the counterflow of the oxidizer and the fuel streams and it is the same kind with the flamelets that has been used extensively in diesel combustion modeling, while the second corresponds to a flamelet that is formed from the counterflow of the combustion products and the fuel streams. Based on the above observations, we can conclude that sets of points in the (Z,J) plane with constant η value should belong in the same flamelet, and as it is shown in [6], these sets are represented geometrically by a straight line in the (Z,J) plane.

Therefore, lines of constant η represent different flamelets, that is, flames that are formed from the counterflow of a fuel stream and different blended EGR-oxidizer streams. The general form of the equation that describes different flamelets in the (Z,J) plane is given by:

$$J = J_{\text{F}_i}\frac{1-Z}{1-Z_{\text{F}_i}}, \qquad i = 1,\ldots,N_{\text{F}}, \qquad (13)$$

where Z_{F_i} and J_{F_i} are the coordinates of the EGR-oxidizer streams at different level of mixing, and N_{F} is the total number of flamelets that are considered. A representative sketch of multiple flamelets in the (Z,J) plane is given in Figure 3.

From the above discussion, it is apparent that different flamelets are created by selecting representative values of the η variable. However, because the orientation of the flamelets in (Z,J) plane is not constant and is not parallel to the Z axis, the corresponding scalar dissipation rate, χ, should be calculated not along the Z axis but along the orientation of each individual flamelet which is determined by the line of constant η. Thus, a natural choice to derive the governing equations of the reactive scalars for each flamelet is the coordinate, Z_i^*, which has the orientation of the flamelet and its relationship to the Z coordinate given by the following equation

$$Z_i^* = \frac{Z - Z_{\text{F}_i}}{1 - Z_{\text{F}_i}}. \qquad (14)$$

Then, by introducing the Z_i^* coordinate into the governing equations of the reactive scalars for the i^{th} flamelet we have

$$\rho\frac{\partial \psi_j}{\partial t} = \rho\frac{\tilde{\chi}_Z}{2}\frac{1}{\left(1-Z_{\text{F}_i}\right)^2}\frac{\partial^2 \psi_j}{\partial Z_i^{*2}} + \omega_j, \qquad (15)$$

where $\tilde{\chi}_Z$ is the conditional Favre mean scalar dissipation rate which is modeled by $\tilde{\chi}_Z = c_\chi \frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{Z''^2}$.

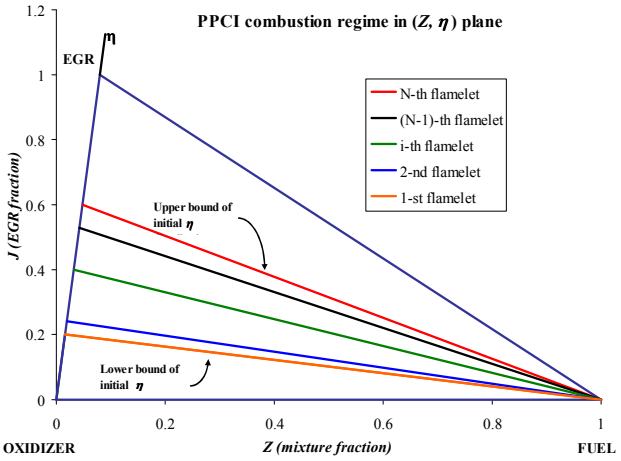

Fig.3, Representation of multiple flamelets in the (Z,η) plane.

Using the properties of variance and the definition of the Z_i^* variable, the relationship of the conditional Favre mean scalar dissipation rate expressed in both coordinates, the mixture fraction, Z, and the normalized mixture fraction, Z_i^*, can be derived as

$$\widetilde{\chi_{Z_i^*}^*} = c_\chi \frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{Z_i^{*2}} = c_\chi \frac{\tilde{\varepsilon}}{\tilde{k}}\frac{\widetilde{Z''^2}}{\left(1-Z_{\text{F}_i}\right)^2} = \tilde{\chi}_Z \frac{1}{\left(1-Z_{\text{F}_i}\right)^2}. \qquad (16)$$

Then, combining equations (15) and (16), the governing equation of the j^{th} reactive scalar, of the i^{th} flamelet based on the Z_i^* coordinate are written as

$$\rho\frac{\partial\psi_j}{\partial t}=\rho\frac{\widetilde{\chi^*_{Z_i^*}}}{2}\frac{\partial^2\psi_j}{\partial Z_i^{*2}}+\omega_j. \qquad (17)$$

Equation (17) has the same functional form with the original governing equation that is used in diesel combustion, with the only difference that the mixture fraction Z is replaced by the normalized mixture fraction Z_i^*, where the normalization factor depends on the individual flamelet.

2.3 The Regenerative Multiple Flamelet (RMF) Model

In the proposed approach, all reactive scalars, ψ_i, are determined as a function of time and the two conserved scalars, Z^* and η i.e., $\psi_i=f_i\left(t,Z^*,\eta\right)=g_i\left(t,Z,J\right)$. However, the function f_i in the preceding expressions does not have the same form over time but it changes when mixing occurs to account for the history effects arising from the nonlinearity of reaction rates.

Before the new model is presented, it is necessary to introduce the coefficient $\alpha_k\left(t,\mathbf{x}\right)$ which represents the fluid mass fraction at $\left(t,\mathbf{x}\right)$ that originated from flamelet k (=1, …,) and it is introduced to determine the mixing of different flamelets on the physical domain. The coefficient $\alpha_k\left(t,\mathbf{x}\right)$ of each flamelet also behaves as a conserved scalar, and thus it satisfies the following transport equation:

$$\bar{\rho}\frac{\partial\alpha_k(t,\mathbf{x})}{\partial t}+\bar{\rho}\tilde{\mathbf{u}}\cdot\nabla\alpha_k(t,\mathbf{x})=\nabla\cdot\left(\bar{\rho}D_t\nabla\alpha_k(t,\mathbf{x})\right), \qquad (18)$$

$k=1,\ldots,N_F$

with $0\le\alpha_k(t,\mathbf{x})\le1$ for $k=1,\ldots,N_F$ and $\sum_{k=1}^{N_F}\alpha_k\left(t,\mathbf{x}\right)=1$. Here D_t is the turbulent diffusivity of the exhaust gases (EGR), which is assumed to be the same for all species, and N_F is the total number of flamelets.

Based on the above, a modified multi-flamelet model the so-called regenerative multiple flamelet (RMF) model, is proposed for the PPCI combustion process. A key feature of the new model is that incorporates the history effect by the following procedure:

Create multiple flamelets based on the interval of the η variable.

Use transport equations to determine their mixing in the physical domain.

At the end of each time step, regenerate a new set of flamelets that are initialized based on the previous ones.

The detailed implementation of the RMF model, is presented in [6].

3 Comparison of the RIF and the RMF strategies

For the preliminary validation of the new approach, a two-dimensional (2DRD) code was developed to solve an incompressible reactive diffusive system in a rectangular domain. Particularly, the code solves the governing equations for the species mass fraction, the energy, the J conserved scalar and the α coefficients. A one-step global CH_4 chemistry with five stable species, CH_4, O_2, N_2, CO_2, H_2O was adopted. The 2D domain was initialized by dividing it into 16 regions, 4 in each direction. Although there were 16 regions, these were initialized by 15 different homogeneous mixtures which have the same equivalence ratio, ϕ = 1, but different EGR levels. The temperature distribution at the start of the calculation is given in Figure 4. For simplicity the mixture fraction was constant in which case the flamelets degenerate into zones (homogeneous reactors). The physical domain was discretized using 51 grid points in each direction while for the RIF and RMF strategies 15 flamelets (zones) where selected. (The number of flamelets represents the selected resolution of the RIF and RMF models)

For the model validation the reactive scalars are computed by using the conserved scalar approach based on the RMF and RIF strategies and compared with their corresponding values obtained by direct integration of the governing equations.

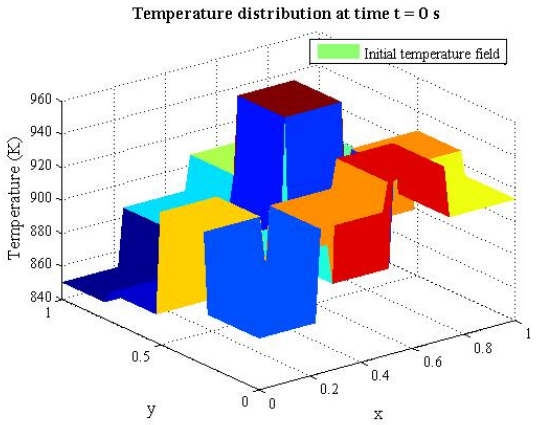

Fig.4, Initial temperature distribution in the physical domain.

In Figures 5 and 6 the temperature fields of the two models are compared to the direct calculation results at time $t = 11.16$ms, when combustion has been completed. By comparing these figures, it is apparent that the RMF model can capture relatively well the actual state of the reactive system, as it predicts the completion of the combustion while the two temperature fields are in a good agreement. On the other hand, the RIF model as illustrated in Figure 6 cannot capture the equilibrium, but based on this the combustion is still incomplete.

4 Conclusions

In the new approach, the PPCI combustion is mapped into the two dimensional (Z,η) space. The η and Z^* conserved variables are newly introduced as functions of the Z and J variables in order to properly represent different flamelets. Based on the proposed representation, the reactive scalars (species mass fractions and enthalpy) are expressed as a function of time and the two conserved scalars. However, the functional dependence changes over time due to the history effects as well as the nonlinearity of chemical reactions. To account for this, the regeneration algorithm which updates the functional representation of the reactive scalars was introduced. Finally, using a simplified CFD code, the comparison of the RIF and the RMF strategies with the direct calculation showed the suitability of the regeneration to account for changes due to nonlinear effects when the conserved scalar approach is used.

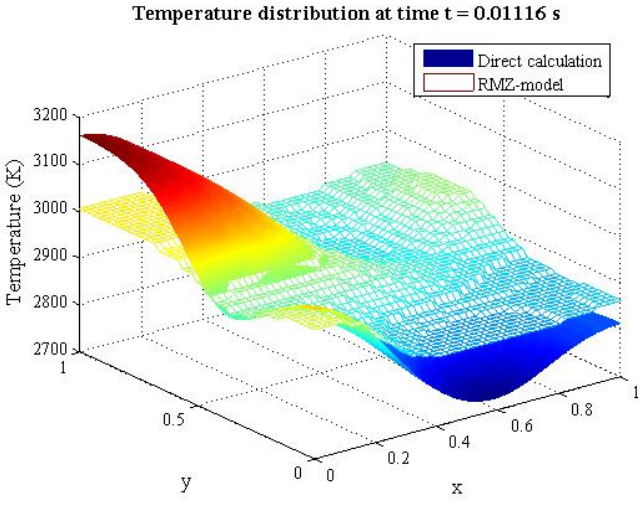

Fig.5, Comparison of the temperature field between the direct calculation and the RMF model with 15 flamelets (zones) at time $t = 11.16$ms, when combustion is completed.

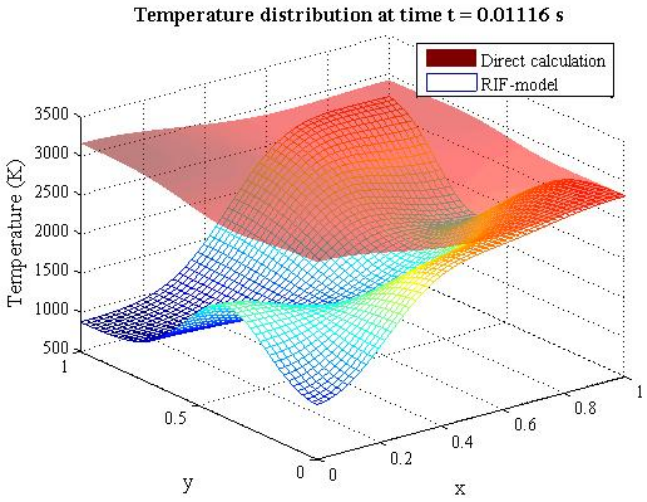

Fig.6, Comparison of the temperature field between the direct calculation and the RIF model with 15 flamelets (zones) at time $t = 11.16$ms, when combustion is completed.

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