Modification of the Temperature Calculation Library for
Premixed Turbulent Combustion Simulation

Ehsan Yasari$^{1,2}$

$^1$ PhD Student at Chalmers University of Technology

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As reviewed elsewhere [1], premixed turbulent combustion occurs often in the flamelet regime, i.e. the probability of finding intermediate (between unburned and burned) states of the mixture is much less than unity everywhere within turbulent flame brush. In such a case, the Reynolds-averaged density $\bar{\rho}$ and the Favre-averaged temperature $\bar{T} \equiv \bar{\rho} \bar{T} / \bar{\rho}$ are determined by the following well-known BML equations [2].

$$\frac{1}{\bar{\rho}} = \frac{1}{\rho_a} \tilde{b} + \frac{1}{\rho_b} (1 - \tilde{b})$$

$$\bar{T} = T_u \tilde{b} + T_g (1 - \tilde{b}) \quad (1)$$

where $\tilde{b}$ is the Favre-averaged regress variable, and subscripts $u$ and $b$ designate unburned and burned mixture, respectively. However, numerical simulations performed by the present author have shown that the Favre-averaged temperature yielded by XiFoam solver using OpenFOAM(1.7.1)’s library differs significantly from $\bar{T}$ calculated using Eq. (1) in the middle part of a turbulent flame brush. The goal of the present work is to stress this problem and to propose a method for resolving it. In OpenFOAM, calculation of temperature (see library janaThermoI.H ) is based on the following equation

$$\frac{hW}{RT} = \frac{H}{RT} = \sum_{i=1}^{\infty} \left( \frac{W}{W_k} Y_k \frac{H_k}{RT} \right) = \sum_{k=1}^{N} \left[ \frac{W}{W_k} Y_k \left( a_{1k} + \frac{a_{2k}}{2} T + \frac{a_{3k}}{3} T^2 + \frac{a_{4k}}{4} T^3 + \frac{a_{5k}}{5} T^4 + \frac{a_{6k}}{6} T \right) \right] \quad (2)$$

where $a_{jk}$ are the JANAF coefficients for the $k$-th specie, $W$ designates molecular weight, $Y_k$ is the mass fraction of the $k$-th specie, and the specific enthalpy $h = H/W$ of the mixture is evaluated by numerically integrating a proper balance equation. While Eq. (2) is well known to hold for a multi-component mixture; in OpenFOAM, this approach is applied to basically different problem, i.e. the intermittency of unburned and burned mixture (separated by a thin flamelet) within turbulent flame brush. More specifically, the mean state of the mixture within the flame brush is considered to be a “super-mixture” of reactants and products, with the mass fractions $Y_1$ and $Y_2$ of reactants and products, respectively, being assumed to be equal to $\tilde{b}$ and $1 - \tilde{b}$, respectively. Accordingly, at first, the molecular weight $W_m$ and JANAF coefficients $a_{jm}$

$^2$ Corresponding Author: Ehsan Yasari (yasari@chalmers.se)
for the super-mixture are determined as follows (see libraries homogeneousMixture.C, janafThermoI.H, specieI.H)

\[
\frac{1}{W_m} = \frac{1}{W_r} \tilde{b} + \frac{1}{W_p} (1-\tilde{b}), \quad \frac{a_{jm}}{W_m} = \frac{a_{jm}}{W_r} \tilde{b} + \frac{a_{jm}}{W_p} (1-\tilde{b})
\]  

(3)

and, then, the Favre-averaged temperature is evaluated using the following equation (see libraries janafThermoI.H, specieThermoI.H)

\[
\tilde{h} \frac{W_m}{RT} = a_{im} + \frac{a_{2m}}{2} \tilde{T} + \frac{a_{3m}}{3} \tilde{T}^2 + \frac{a_{4m}}{4} \tilde{T}^3 + \frac{a_{5m}}{5} \tilde{T}^4 + \frac{a_{6m}}{6} \tilde{T}
\]  

(4)

However, such an approach suffers from two flaws, at least. First, multi-component gas mixture and reactant-product intermittency within turbulent flame brush are two totally different phenomena and there are no justification for applying Eq. (2) to the super-mixture. For instance, all species of a multi-component gas have the same temperature, whereas \( T_r \neq T_p \) as far as the reactant-product intermittency is concerned. Second, the non-linear Eq. (2) does not commute with taking a mean, i.e. substitution of \( \bar{\rho} \tilde{T}^n / \bar{\rho} \) with \( \tilde{T}^n \) in the averaged Eq. (2) results in substantial errors.

To resolve the problem, the following method of evaluating \( \tilde{T} \) was implemented into the library hhuMixtureThermo.C of OpenFOAM. First, based on the local value of \( \tilde{h} \) obtained by numerically integrating a proper balance equation, the local values of \( T_u \) and \( T_b \) are determined by applying Eq. (2) to pure reactants and pure products, respectively, i.e. \( T_u \) (\( T_b \)) is calculated using the reactant (product) JANAF coefficients (see hhuMixtureThermo.C). Second, the Favre-averaged temperature is computed using Eq. (1).

In order to compare the original and modified methods of calculating \( \tilde{T} \), the following relative error

\[
\delta \rho(t) \equiv \max \left| \frac{\rho_{OF}(x,t) - \bar{\rho}(x,t)}{\bar{\rho}(x,t)} \right|
\]  

(5)

was determined. Here, \( \rho_{OF} \) is the mean density yielded by the original OpenFOAM, \( \bar{\rho} \) is evaluated using Eq. (1), and the maximum is found in space at each time step. Typical results are shown in Fig. (1). As it can be seen, for the modified approach this value is much smaller which proved that this approach is correct. Fig. (2) shows the variation of radius versus time for the range of laminar flame speed between 0.1-0.4 m/s. It is shown that by increasing the laminar flame speed the flame propagating rate is increased.

REFERENCES
