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Self-similar behavior and chemistry tabulation of burnt-gas diluted premixed flamelets including heat-loss

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In many combustion systems, the reactive gases feeding the reaction zones are diluted by burnt products, to favor flame stabilization, homogenize the temperature distribution and reduce pollutant emission. The objective of this paper is to discuss a premixed flamelet detailed chemistry tabulation strategy for vitiated and non-adiabatic combustion. Dilution by burnt products is parameterized here with two controlling quantities: the amplitude of the heat-loss in the burnt gases, for instance at walls, and the level of reactant vitiation. The chemical response of premixed flames to variations of these parameters is studied and it is shown that most chemical properties of burnt-gas diluted flames feature self-similar behavior, which can be used to dramatically downsize chemical tables based on canonical flamelets. The self-similar behavior of the flamelets is studied for both molecular diffusion and chemical source budgets in a progress variable composition space. It is found that two different scaling relations are needed to ensure self-similar behavior of both major and radical species.

Keywords: self-similar flame behavior; detailed chemistry tabulation; burnt-gas dilution; non-adiabatic combustion; flame simulation

1. Introduction

In many combustion systems, the gases feeding the reaction zones are not exclusively composed of fresh fuel and oxidizer; instead some degree of dilution by burnt products exists. The recirculating hot products contain thermal energy that may be useful to favor flame stabilization. Dilution by burnt gases also tends to reduce temperature gradients by homogenizing the mixture, and high temperature levels associated with NOx production are then lessened. In laboratory jet-flames, burnt products sent in a nonflowing stream are used to stabilize combustion or to mimic dilution effects [1, 2]. In swirling burners, flame stabilization can be influenced easily by burnt gases circulating within the swirling motion [3, 4]. Even in flames lifted above the fresh fuel and oxidizer without vitiated coflow, combustion on the fuel-rich side was found to be influenced by upstream products formed at the turbulent flame base [5–7]. In large scale systems such as furnaces, burnt gases contribute to flame stability in various ways, and for high levels of flame dilution by-products, the moderate or intense low-oxygen dilution (MILD) [8] or the flameless regime are observed [9, 10]. The enthalpy of combustion products may vary in real systems depending

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on the amount of heat transferred at the walls by these recirculating products or because of radiative effects. Hence, dilution by burnt gases strongly influences turbulent combustion in many ways and profoundly affects the thermochemical properties of the mixture entering the reaction zones. Nevertheless, most turbulent combustion models implicitly formulate the hypothesis that the unburned reactants are composed of fresh fuel and oxidizer [11–13].

Detailed combustion chemistry needs to be reduced or tabulated before its introduction in turbulent flame simulations [14]. The objective of this paper is to discuss a premixed flamelet detailed chemistry tabulation strategy for burnt-gas diluted and non-adiabatic premixed combustion. In particular, it is intended to take advantage of self-similar properties of these flamelets to reduce the size of chemical look-up tables, prior to their introduction in flow solvers grounded on massively parallel computing. However, it is not intended to examine regimes approaching flameless combustion; instead, care is taken to ensure that a propagating flame front can always develop for the considered composition and temperature of the unburned mixture. This constraint limits the maximum level of dilution by burnt gases that is considered, the focus being intentionally restricted to diluted premixed flamelets only.

The starting point is the self-similar flamelet tabulation technique originally proposed by Ribert et al. [15] for non-diluted laminar premixed flames. This approach is extended here to burnt-gas diluted flames including heat-loss. These flamelet based tabulations have been previously associated with a presumed probability density function to simulate premixed and non-premixed turbulent flames, both in the Reynolds Average Navier–Stokes (RANS) and Large-Eddy Simulation (LES) contexts [16–20]. Recently, these detailed chemistry tabulation approaches were extended to partially premixed combustion [21]. An attempt to deal with non-adiabatic combustion was made, building the tabulation from premixed laminar and attached burner flames [22,23], but this former approach was found to be short of flexibility, because of the specific laminar burner configuration, which does not allow for the introduction of dilution by burnt gases with an easy control of both enthalpy and unburned gas composition. In the formalism discussed below, both dilution and enthalpy variations are examined to mimic real flow behavior, then the self-similar properties of the resulting methane–air flamelets are investigated.

The next section describes the flame model problem and the parameters that are retained. Then, flame responses to dilution for various enthalpy levels are studied; the subsequent section reports on the self-similar behavior of burnt-gas diluted combustion and how detailed chemistry tabulation strategies can be derived from this observation. It is important to note that the detailed chemical scheme used throughout the paper (GRI-3 [24]) has not been specifically developed for burnt-gas vitiated combustion; the exact values of species concentration can therefore be questioned. Nevertheless, it is legitimate to investigate the global self-similar behavior and the demonstration of the tabulation technique, even if some details of the chemistry would need adjustments for being fully predictive in a vitiated environment. This method can be readily applied to any detailed chemical scheme.

2. Model problem for premixed burnt-gas diluted combustion

One-dimensional canonical combustion problems have been widely used to understand basic flame behaviors and tabulate the chemistry in the framework of flamelet modeling [14, 25]. In such one-dimensional flow, any thermochemical variable \( \varphi(x, t) \) satisfies a balance equation that reads,

\[
\frac{\partial \rho \varphi}{\partial t} = \frac{\partial F_x(\varphi)}{\partial x} + \dot{\omega}_\varphi
\]  

(1)
where $F_x(\varphi)$ is the budget of $\varphi$-fluxes in $x$-space. In premixed flamelets with non-unit Lewis numbers,

$$F_x(\varphi) = (-u + V_\varphi) \rho \varphi \tag{2}$$

where $u$ is the flow velocity and $V_\varphi$ the molecular diffusion velocity of the $\varphi$ variable. For the boundary conditions: $\varphi(-\infty) = \varphi^u$, denoting a premixed fresh mixture flowing at velocity $u(-\infty)$, and $\varphi(+\infty) = \varphi^b$ the corresponding fully burnt gases, a steady one-dimensional premixed flame propagating at speed $S_L = u(-\infty)$ may be obtained. In the following, only freely propagating steady flamelets are considered, hence the flame is not subjected to an external strain that would be induced by an imposed velocity gradient. Three free parameters are chosen to characterize the unburnt-gas conditions $\varphi^u(\phi, \alpha, \beta)$. The first, $\phi$, is the fuel–air equivalence ratio of the mixture; the second, $\alpha$, is the dilution rate of the pure reactants with burnt gases; and the third, $\beta$, is a heat-loss factor applied to the products before their mixing with fresh gases to complete dilution.

The dilution rate $\alpha$ is defined as the ratio of the mass of products diluting fresh gases to the total mass of unburned gases, so that the unburned mass fraction $Y^u_k$ of the $k$-th species may be written:

$$Y^u_k(\phi, \alpha, T^u) = (1 - \alpha)Y^f_k(\phi, T^f) + \alpha Y^p_k(\phi, T^p) \tag{3}$$

where $Y^f_k(\phi, T^f)$ is the undiluted fresh reactant composition at fuel–air equivalence ratio $\phi$ at temperature $T^f = 297$ K, $Y^p_k(\phi, T^p)$ is the composition of the circulating products at temperature $T^p$ obtained from chemical equilibrium calculations. In Equation (3), the dependence on the heat-loss factor $\beta$ was implicitly expressed in terms of the temperature $T^p$, which is easily related to $\beta$ via the enthalpy quantifying the thermal part of the problem.

$$H^f(\phi, T^f) = \sum_{k=1}^{N} Y^f_k(\phi, T^f) h_k(T^f)$$

is the enthalpy of the fresh reactants, with $h_k$ the total enthalpy of the $k$-th species, and

$$H^p(\phi, T^p) = \sum_{k=1}^{N} Y^p_k(\phi, T^p) h_k(T^p)$$

the enthalpy of the products at temperature $T^p$, which may differ from $T^{Eq}$, the equilibrium temperature, because of heat-loss. The enthalpy of the diluted mixture then reads:

$$H^u(\phi, \alpha, T^u) = (1 - \alpha)H^f(\phi, T^f) + \alpha H^p(\phi, T^p) \tag{4}$$

where $H^p(\phi, T^p)$, the burnt products enthalpy at $T^p$, is expressed from $H^p(\phi, T^{Eq})$, the products enthalpy under adiabatic conditions to which a heat-loss of amount $Q_W$ is applied,

$$H^p(\phi, T^p) = H^p(\phi, T^{Eq}) - Q_W. \tag{5}$$

Here $Q_W$ represents energy transfer at the walls and/or radiation in a real system. Because combustion of mixed fresh and burnt gases is assumed, through an adiabatic premixed flame before any heat-loss to occur, $H^u(\phi, \alpha, T^u) = H^p(\phi, T^{Eq})$, then

$$Q_W = H^u(\phi, \alpha, T^u) - H^p(\phi, T^p) = (1 - \alpha)[H^f(\phi, T^f) - H^p(\phi, T^p)] \tag{6}$$
Figure 1. Sketch of the chemistry tabulation parameters, see Equations (3)–(8).

which is parameterized from the $\beta$ factor,

$$\beta = \frac{H^f(\phi, T^f) - H^p(\phi, T^p)}{H^f(\phi, T^f) - H^p(\phi, T^f)}$$

leading to

$$Q_W = \beta(1 - \alpha)(H^f(\phi, T^f) - H^p(\phi, T^f)).$$

For $\beta = 0$, there is no heat-loss ($Q_W = 0$) and $T^p = T^\text{Eq}$ (adiabatic combustion); for $\beta = 1$, the heat-loss is maximum and $T^p = T^f$. Figure 1 illustrates this parameterization of burnt-gas diluted flames.

The fresh and burnt temperatures of a methane–air mixture given by Equations (3) and (4) are given in Figure 2 for a stoichiometric chemical composition computed with the 53-species thermochemistry of the GRI-3 [24] mechanism. As expected, without heat-loss the methane–air adiabatic combustion temperature ($\simeq 2200$ K) is recovered for every dilution rate $\alpha$. For a given non-zero $\alpha$, by increasing $\beta$, the heat-loss factor, both the unburned and burnt temperatures decrease. Also for non-zero $\beta$, the higher the dilution rate, the lower is the burnt-gas temperature. Similar trends are observed for non-unit equivalence ratio. This result goes in the direction of trends observed in flameless combustion [8]: to minimize the temperature jump between the burnt and unburned mixture both dilution and heat-loss are necessary.

Eight-hundred and twenty-five methane–air flames have been simulated with the software package PREMIX [26] using the GRI-3 [24] detailed chemistry mechanism including differential diffusion for: three values of the equivalence ratio ($\phi = 0.7; 1.0; 1.4$); 25 values of the dilution rate ($0.0 \leq \alpha \leq 0.24$); and 11 values of the heat-loss factor ($0.0 \leq \beta \leq 1.0$). As alluded to in the Introduction, the dilution rate is limited to $\alpha \leq 0.24$, to stay within a combustion regime with propagating flames. This limit was set so that the most vitiated unburned mixture features an ignition delay large enough to prevent self-ignition to be the only driving mechanism; the fact that the mixture cannot self-ignite when convected over a length of 100 m at a typical flame speed was used as the criterion.
The analysis of this database is reported thereafter from 20 representative cases summarized in Table 1. The combustion is under constant pressure, the one-dimensional coordinate through the simulated flame extends over $x \in [-100, 100]$ in meters with non-uniform mesh spacing, to avoid perturbations from inlet and outlet conditions and to permit chemical equilibrium to be reached in the burnt gases.

Table 1. Flame parameters (see Equations 3 and 4).

<table>
<thead>
<tr>
<th>Case</th>
<th>$\phi$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
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<tr>
<td>(ii)</td>
<td>0.7</td>
<td>0.16</td>
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<tr>
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<td>0.7</td>
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<tr>
<td>(ix)</td>
<td>1.4</td>
<td>0.24</td>
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<tr>
<td>(xi)</td>
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<td>0.2</td>
<td>0.5</td>
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<tr>
<td>(xii)</td>
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3. Premixed flame response to dilution by burnt gases

Before discussing the self-similar structure of burnt-gas diluted flames, the responses to dilution of global flame properties, which are ingredients of the self-similar flame solutions, are summarized.

3.1. Impact of dilution on equivalence ratio

A preliminary and simple point must be made concerning the definition of equivalence ratio. The atomic concentration in carbon, oxygen, hydrogen and nitrogen is fixed in the problem considered (i.e. premixed flamelets), aside from a very small deviation induced by differential diffusion, which may be observed across the flame. Formally, for a given carbon–oxygen ratio, the fuel–oxygen mass ratio may vary; as also the equivalence ratio, which is this ratio normalized by its stoichiometric value. If the fresh fuel and oxidizer mixture is lean or rich, dilution by burnt gases of the same mixture will not cause the atomic ratio to vary, but the equivalence mass ratio of the diluted unburned reactants will be different from that of the fresh ones, with direct effects on the chemistry.

Let us consider the global reaction,

\[ v_F F + v_O O \rightarrow v_P P \]  (9)

which summarizes all the elementary steps of the detailed kinetics. The stoichiometric mass ratio of the mixture is:

\[ s = \frac{v_O W_O}{v_F W_F} \]  (10)

where \( W_k \) is the molar weight of species ‘\( k \)’. In the case of a lean mixture, the oxidizer mass fraction may be written:

\[ Y_{O,o} = s Y_{F,o} + \kappa_O. \]  (11)

The equivalence ratio then reads:

\[ \phi = \frac{Y_{F,o}}{Y_{O,o}} s = \frac{1}{1 + \kappa_O/(s Y_{F,o})} \]  (12)

where \( \kappa_O = 0 \) corresponds to the stoichiometric condition. For \( \kappa_O > 0 \), the mixture is lean, \( \phi < 1 \), and a mass fraction \( \kappa_O \) of oxidizer is found in the products. In the case of a rich mixture, the fuel mass fraction may be written:

\[ Y_{F,o} = \frac{1}{s} Y_{O,o} + \kappa_F. \]  (13)

The equivalence ratio then reads:

\[ \phi = \frac{Y_{F,o}}{Y_{O,o}} s = 1 + s \frac{\kappa_F}{Y_{O,o}} \]  (14)

where \( \kappa_F = 0 \) corresponds to the stoichiometric condition. For \( \kappa_F > 0 \), the mixture is rich, \( \phi > 1 \), and a mass fraction \( \kappa_F \) of fuel is found in the products.
Let us also now introduce $\alpha$, the dilution ratio between the fresh and burnt gases. The composition of the burnt-gas diluted mixture may be written:

$$\frac{(1 - \alpha)[Y_{F,o} + Y_{O,o}] + \alpha [Y_p + \kappa_k]}{1 - \alpha/s} = 1.$$  \hspace{1cm} (15)

In the lean case, with Equation (11), both the fuel mass fraction, $Y^L_{F,D}$, and the oxidizer mass fraction, $Y^L_{O,D}$, in the diluted unburned mixture, can be determined from Equation (15) as:

$$Y^L_{F,D} = (1 - \alpha)Y_{F,o}$$ \hspace{1cm} (16)

$$Y^L_{O,D} = (1 - \alpha)Y_{F,o}s + \kappa_O.$$ \hspace{1cm} (17)

Then the equivalence ratio is:

$$\phi^L_D = \frac{(1 - \alpha)Y_{F,o} s}{1 - \alpha/s + \kappa_O/(sY_{F,o})}.$$ \hspace{1cm} (18)

The equivalence ratio of the entering fresh mixture, $\phi$, and the equivalence ratio of the burning mixture, $\phi^L_D$, are related by:

$$\phi^L_D = \frac{(1 - \alpha)\phi}{1 - \alpha \phi}.$$ \hspace{1cm} (19)

In the rich case, introducing Equation (13), both the fuel mass fraction, $Y^R_{F,D}$, and the oxidizer mass fraction, $Y^R_{O,D}$, in the diluted unburned mixture can be determined from Equation (15) as:

$$Y^R_{F,D} = \frac{1 - \alpha}{s} Y_{O,o} + \kappa_F$$ \hspace{1cm} (20)

$$Y^R_{O,D} = (1 - \alpha)Y_{O,o}.$$ \hspace{1cm} (21)

Then the equivalence ratio is:

$$\phi^R_D = \frac{(1 - \alpha)Y_{O,o}/s + \kappa_F}{(1 - \alpha)Y_{O,o} s} = \frac{1 - \alpha + s\kappa_F/Y_{O,o}}{1 - \alpha}.$$ \hspace{1cm} (22)

The equivalence ratio of the entering fresh mixture, $\phi$, and the equivalence ratio of the burning mixture, $\phi^R_D$, are related by:

$$\phi^R_D = \frac{\phi - \alpha}{1 - \alpha}.$$ \hspace{1cm} (23)

Figure 3 displays the behavior of the diluted equivalence ratio for various dilution ratios $\alpha$ and equivalence ratios of the fresh mixture. The variation of equivalence ratio is not completely negligible; this must be kept in mind when analyzing the flame response for various $\alpha$, as discussed now.
3.2. Global flame behavior

As the dilution rate $\alpha$ changes, both the flame speed $S_L$, and the flame thickness, $\delta_L$, of the diluted premixed flame evolve. Figure 4(a) shows profiles of flame speed $S_L$, as a function of dilution rate $\alpha$, for the lean, stoichiometric and rich cases of adiabatic diluted premixed flames. Increasing $\alpha$ leads to larger flame speeds, as the amount of thermal energy in the fresh gases has increased, for the case $\phi = 1$, $S_L > 1$ m s$^{-1}$ for $\alpha > 0.17$. Dilution by burnt gases also compensates the flame speed decrease induced by departure of the equivalence ratio from stoichiometry; for instance a non-diluted stoichiometric flame and a lean ($\phi = 0.7$) flame 12% diluted have approximately the same flame speed, a simple observation that may be of interest in flame stabilization studies.

To calibrate the mesh resolution in numerical simulation of turbulent flames, the thermal flame thickness and the reaction zone thickness are essential ingredients. Two estimations of flame thickness are used, i.e. the thermal thickness,

$$\delta_T = \frac{T_{\text{max}} - T_{\text{min}}}{(dT/dx)_{\text{max}}}$$  \hspace{1cm} (24)$$

and the reaction zone thickness $\delta_k$ of the $k$-th species

$$\delta_k = x_k^2 - x_k^1,$$  \hspace{1cm} (25)$$

$x_k^1$ and $x_k^2$ represent the first and second locations, respectively, where the $k$-th species reaction rate reaches half of its maximum value. The species reaction zone thickness $\delta_{\text{CH}_4}$ increases slightly as the dilution rate increases, see Figure 4(c). On the contrary, Figure 4(b) shows that the flame thermal thickness $\delta_T$ decreases as the dilution rate increases. Increasing the dilution rate leads to a decrease of both the temperature range $\Delta T = T_{\text{max}} - T_{\text{min}}$ and the maximum temperature gradient $(dT/dx)_{\text{max}}$, as shown in Figure 4(d) for the rich case.
Figure 4. $\beta = 0$: (a) flame speed, (b) thermal thickness, (c) reaction zone thickness. Solid: $\phi = 0,7$; dot: $\phi = 1,0$; dash: $\phi = 1,4$; (d) $\phi = 1,4$, dot dash: $(T_{\text{max}} - T_{\text{min}})/(T_{\text{max}} - T_{\text{min}})_{\alpha = 0}$; double-dot dash: $(dT/dx)^{\text{max}}/(dT/dx)_{\alpha = 0}$.

$\phi = 1,4$, where profiles are normalized by their corresponding values under the undiluted condition. Since the temperature range decreases much more quickly than the maximum temperature gradient, the flame thermal thickness (Equation 24) decreases as the dilution rate increases.

The amount of heat-loss, and thus the enthalpy level, also influences the diluted flame response. Figure 5(a) shows the flame speed, $S_L$, as a function of heat-loss factor $\beta$, for the lean, stoichiometric and rich cases of non-adiabatic diluted premixed flames, with a dilution factor $\alpha = 0,2$. As expected, the flame speed decreases as the heat-loss factor $\beta$ increases. The fuel reaction zone thickness becomes wider for higher level of heat-loss (Figure 5c), agreeing with the behavior of the thermal thickness $\delta_T$, as shown in Figure 5(b). As the heat-loss factor $\beta$ increases, both the temperature range $\Delta T$ and the maximum temperature gradient $(dT/dx)^{\text{max}}$ increase (Figure 5d). The temperature range $\Delta T$, however, increases much more quickly than the maximum temperature gradient $(dT/dx)^{\text{max}}$. Therefore, the flame thermal thickness $\delta_T$ increases as the heat-loss factor $\beta$ increases. This trend, which could lead to reaction zones spreading over large flow volumes, as seen in flameless combustion, appears in this study to be associated to non-negligible heat-loss.

When both the amount of dilution and the heat-loss evolve, the responses of global flame properties become more complex (Figures 6a and 7a). For flames with a low heat-loss factor, the flame speed increases with dilution rate. For heat-loss factor larger than 0,6, heating
of fresh reactants by burnt products becomes less effective and the heat-ballast effect of burnt gases becomes dominant; a large part of the heat released by exothermic reactions is then used to heat the products, and the flame speed decreases. The maximum flame speed is found for the adiabatic flame ($\beta = 0$), with the highest dilution rate ($\alpha = 0.24$), while the minimum flame speed is found for the diluted flame with maximum heat-loss ($\beta = 1$) and still the highest dilution rate. The thickness of the fuel reaction zone increases with either dilution rate or heat-loss factor (Figures 6c and 7b). The maximum reaction zone thickness is found for a diluted flame with $\beta = 1$ and $\alpha = 0.24$. Figure 6(b) shows that the tendency of the thermal flame thickness response to dilution rate and heat-loss factor is similar to that of the reaction zone thickness, except close to the adiabatic condition, where the thermal flame thickness decreases with increasing dilution rate, as shown in Figure 4(b). This is because, close to the adiabatic condition, the temperature range $\Delta T$ decreases more quickly than the maximum temperature gradient $(dT/dx)_{\text{max}}$, as the dilution rate increases (Figure 6d).

### 3.3. Major and minor species distribution

The impact of variations in $\alpha$ and $\beta$ on representative species distributions is shown in Figures 8 and 9 for cases (xiii)–(xv) and (xix) of Table 1. By definition, in an unburned mixture diluted by burnt products, the fresh-gas temperature, CO$_2$ and H$_2$O mass fractions
increase, while the CH₄ and O₂ mass fractions decrease; the equilibrium temperature and species mass fractions are, however, unchanged by dilution with β = 0 (Figures 8a and 8c). The peak value of the CO mass fraction decreases slightly with adiabatic dilution, while those of the O and OH mass fractions increase slightly (Figures 8b and 8d). Introducing heat-loss (Figures 9a, 9c and 8c), the fresh gases and equilibrium temperature are lower, and equilibrium mass fractions also differ. Comparing Figures 9(b)–9(d) and 8(d), the peak value of minor species mass fractions decreases considerably due to heat-loss, because of the reduction in species dissociation. This is confirmed by representative species reaction rates (Figures 10 and 11). All major and minor species reaction rates change slightly due to adiabatic dilution (Figures 10a and 10d). The species reaction rates, however, decrease significantly as the heat-loss increases, as shown in Figures 11(a) and 11(d).

4. Self-similar premixed diluted combustion and detailed chemistry tabulation

4.1. Self-similar composition space formalism

Self-similar flame tabulation (S2FT) was introduced by Ribert et al. [15] to reduce the memory size required to store flamelet libraries on massively parallel computers. In the usual tabulation techniques [21,25,27], chemical source terms, or species mass fractions, are extracted from laminar premixed flame calculations and stored versus appropriate variables. For example, if such libraries are composed of flames at various equivalence ratios φ, a
mixture fraction must be defined as a coordinate of the look-up table in addition to a progress variable $Y_c$. Increasing the number of tabulated parameters, such as the pressure $P$, inlet temperature $T_f$, dilution rate $\alpha$, heat-loss $\beta$, etc. may lead to very large databases. Adding 10 dilution levels to a given table would increase its size by a factor 10, making it difficult to use in massively parallel computations. Ribert et al. [15] have proposed taking advantage of the self-similar behavior of one-dimensional laminar premixed flames, replacing an initial two-dimensional database, with $\phi$ and $Y_c$ as coordinates, by four one-dimensional databases, thus saving memory space and access time. This approach was then extended to lookup tables averaged with presumed probability density functions [28], to include the effects of unresolved fluctuations in RANS or LES.

Self-similar behavior was first obtained in physical space [15], but it may also be derived in composition space (the full set of aero-thermochemistry equations in a given composition space may be found in [21]). Using the composition space similarity behavior instead of the...
Figure 8. Major and minor species distribution, \( \phi = 1.0 \). (a), (b): case (xix); (c), (d): case (xiii); (a), (c) Solid line: temperature; dot line: \( Y_{\text{CH}_4} \); dash line: \( Y_{\text{O}_2} \); dot dash line: \( Y_{\text{CO}_2} \); double-dot dash line: \( Y_{\text{H}_2\text{O}} \); (b), (d) solid line: \( Y_{\text{CO}} \); Dot line: \( Y_{\text{O}} \times 10 \); dash line: \( Y_{\text{OH}} \).

physical space behavior, allows for refining the analysis of the various terms contributing to flame evolution versus dilution and heat-loss, as shown below.

With the relation \( \partial / \partial x = \sigma_c \partial / \partial Y_c \), where \( \sigma_c = \partial Y_c / \partial x \), Equation (1) becomes, in the flame reference frame,

\[
\rho_u S_L \sigma_c \frac{\partial Y_k}{\partial Y_c} = \sigma_c \frac{\partial}{\partial Y_c} \left( \rho D_k \sigma_c \frac{\partial Y_k}{\partial Y_c} \right) + \dot{\omega}_k
\]

(26)

where the usual notation is adopted, and \( D_k \) and \( \dot{\omega}_k \) are the diffusion coefficient and the chemical source of the \( k \)-th species. In the present study, where fresh gases are diluted by combustion products, multiple options exist to quantify the progress of reaction; here \( Y_c \) is defined as \( Y_c = (Y_{\text{CO}_2} + Y_{\text{CO}}) - (Y_{\text{CO}_2} + Y_{\text{CO}})^{\nu} \). This expression ensures a monotonic evolution of \( Y_c \) in physical space and a unique correspondence between species, temperature and \( Y_c \). A formal analysis of the one-dimensional composition space flame equation is discussed, leading to a first set of relations and definition of reduced coordinates; coordinates better suited for self-similar behavior of diluted flames are then proposed.
Figure 9. Major and minor species distribution, $\phi = 1.0$. (a), (b): case (xiv); (c), (d): case (xv). (a), (c) Solid line: temperature; dot line: $Y_{\text{CH}_4}$; dash line: $Y_{\text{O}_2}$; Dot dash line: $Y_{\text{CO}_2}$; double-dot dash line: $Y_{\text{H}_2\text{O}}$; (b), (d) solid line: $Y_{\text{CO}}$; dot line: $Y_{\text{O}} \times 10$; dash line: $Y_{\text{OH}}$.

A reduced progress of reaction, defined as

$$Y_{k,c}^+ = \int_0^Y e \frac{\rho_u S_L}{\rho D_k \sigma_e} dY_c,$$

(27)

is introduced into Equation (26), leading to:

$$\frac{\partial Y_k}{\partial Y_{k,c}^+} = \frac{\partial}{\partial Y_{k,c}^+} \left( \frac{\partial Y_k}{\partial Y_{k,c}^+} \right) + \frac{\rho D_k \dot{\omega}_k}{(\rho_u S_L)^2}. $$

(28)

A reduced source term $\dot{\omega}_k^+$,

$$\dot{\omega}_k^+ = \frac{\rho D_k \dot{\omega}_k}{(\rho_u S_L)^2 \Omega_k} \quad \text{with} \quad \Omega_k = \frac{\max(|\rho D_k \dot{\omega}_k|)}{(\rho_u S_L)^2},$$

(29)
as well as a reduced species mass fraction $Y_k^+$,

$$\dot{Y}_k^+ = \frac{Y_k - Y_k^u}{\Omega_k}, \quad (30)$$

are then defined to rewrite Equation (28) as:

$$\frac{\partial Y_k^+}{\partial Y_{k,c}^+} = \frac{\partial}{\partial Y_{k,c}^+} \left( C \frac{\partial Y_k^+}{\partial Y_{k,c}^+} \right) + \dot{\omega}_k^+, \quad (31)$$

with $C = 1$. In practice, it is found that the numerical calculation of $Y_k^+$ according to Equation (27) is sensitive to the starting point of integration, because close to $Y_{k,c}^+ = 0$, the progress variable gradient $\sigma_c$ also approaches zero, which causes numerical errors and leads to a relative shift of the flame along the $Y_{k,c}^+$ coordinate. To avoid this, the definition
of Equation (27) is first improved as:

\[ Y_{k,c}^+ = \int_0^{Y_k} \frac{\rho_{\infty} S_{L}}{\rho D_k \sigma_c} dY_c - Y_{k,c,s}^+ \]  

(32)

where \( Y_{k,c,s}^+ \) is the value of the integral \( \int_0^{Y_k} [\frac{(\rho_{\infty} S_{L})}{(\rho D_k \sigma_c)}] dY_c \) at \( \dot{\omega}_k^+ = 1 \). For this new definition, Equation (29) still holds.

The boundary conditions are given by:

\[ Y_k^+(Y_{k,c} = Y_{k,c}^{\text{min}}) = 0 \quad \text{and} \quad Y_k^+(Y_{k,c} = Y_{k,c}^{\text{max}}) = \frac{1}{\rho_{\infty} S_{L} \Omega_k} \int_0^{Y_k^+} \frac{\dot{\omega}_k}{\sigma_c} dY_c. \]  

(33)

Equation (31) is self-similar if \( \dot{\omega}_k^+ \) depends on \( Y_{k,c}^+ \) only, but not on the flame parameters \( \phi, \alpha, \beta \). This point is analyzed in Figures 12 and 13 for which the reduced convection, diffusion and source terms of Equation (31) are plotted as a function of \( Y_{k,c}^+ \) for \( O_2 \) and \( CH \) species, cases (iv)–(vi) of Table 1. It is found that the source term \( \dot{\omega}_k^+ \) is not exactly self-similar for both major species and \( CH \) radical. Its profile becomes wider as the dilution
rate $\alpha$ increases. The profiles of the reduced gradient, the diffusion term and reduced species mass fraction also enlarge with higher dilution rate. This is consistent with the scattering of reduced source term profiles, as noticed in [15] in the study of self-similar behavior in physical space. Figures 12 and 13 suggest that the extrema reached by either the reduced gradient $\partial Y_k^+ / \partial Y_{k,c}^+$ or the reduced species mass fraction get larger with an increase of dilution by burnt products. With this first set of scaling relations (set 1 of Table 2), an imperfect self-similar behavior is thus observed; other possible scaling relations will now be explored.

The definition of the reduced variables used in Equation (31) can be replaced by a new set of scaling relations summarized in Table 2. The quantities $\delta$ (set 2) and $\delta'$ (set 3) defined as

$$
\delta = Y_{k,c}^2 - Y_{k,c}^1 \quad (34)
$$
$$
\delta' = Y_{Y,k,c}^2 - Y_{Y,k,c}^1 \quad (35)
$$

measure the half-height width of the reaction rate $\dot{\omega}_k$ and the half-height width of the species mass fraction $Y_k$ profile, respectively, in $Y_c$-composition space, as illustrated in Figure 14. For the reaction rate profile with more than one peak, the half-height of the first positive peak will be chosen. For species profiles monotonically increasing or decreasing, $Y_{Y,k,c}^1$ is set to zero and $Y_{Y,k,c}^2$ records the single half-height location in composition space. The species mass fraction is reduced using its maximum and minimum values (see $Y_k^+$

Figure 12. $O_2$ self-similarity (Equations 30 and 31), $\phi = 1.0$. Solid line: case (iv); dot line: case (v); dash line: case (vi).
in Table 2), and $\sigma_{k,c}^+ = \partial Y_c^+ / \partial x = \sigma_c / \delta$ or $\sigma_{k,k,c}^+ = \sigma_c / \delta'$ are introduced modifying the expression for $C$ and $\dot{\omega}_{k,c}^+$ in Equation (31) (Table 2).

For set 2 of Table 2 based on $\delta$ (Equation 34), Figures 15 and 16 display profiles of the reduced gradient $\partial Y_k^+ / \partial Y_{k,c}^+$, the diffusive term of Equation (31), the source terms, and the reduced species mass fraction $Y_k^+$ for the radical CH and major species $O_2$. For the CH radical, the scaling seems appropriate with only small discrepancies in the diffusion and source terms. Moreover, these departures from self-similar evolution cancel with each other, if diffusive and source terms are added. The $O_2$ behavior (Figure 16) is self-similar as far as the source term is concerned. However, a departure from self-similarity is visible on the unburned side.

Table 2. Scaling relations used in Equation (31).

<table>
<thead>
<tr>
<th>Set</th>
<th>$Y_c^+$</th>
<th>$Y_k^+$</th>
<th>$C$</th>
<th>$\dot{\omega}_{k,c}^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set 1</td>
<td>$\int_0^{Y_c} \frac{\rho_u S_k}{\rho D_k \sigma_c} dY_c$</td>
<td>$\frac{Y_k - Y_k^m}{\Omega_k - Y_k^m}$</td>
<td>1</td>
<td>$\frac{\rho D_k \dot{\omega}_k}{\left(\rho_u S_k\right)^2 \Omega_k}$</td>
</tr>
<tr>
<td>Set 2</td>
<td>$\frac{1}{\delta} (Y_c - Y_{k,c}^1)$</td>
<td>$\frac{Y_k^\text{max} - Y_k^\text{min}}{Y_k^\text{max} - Y_k^\text{min}}$</td>
<td>$\frac{\rho D_k}{\rho S_k \sigma_{k,c}}$</td>
<td>$\frac{\rho D_k}{\rho S_k \sigma_{k,k,c}}$</td>
</tr>
<tr>
<td>Set 3</td>
<td>$\frac{1}{\delta} (Y_c - Y_{k,c}^1)$</td>
<td>$\frac{Y_k^\text{max} - Y_k^\text{min}}{Y_k^\text{max} - Y_k^\text{min}}$</td>
<td>$\frac{1}{\rho S_k \sigma_{k,k,c}}$</td>
<td>$\frac{1}{\rho S_k \Delta \sigma_{k,k,c}}$</td>
</tr>
</tbody>
</table>
Figure 14. Profiles of the source term (solid line) and of the mass fraction (dashed line) of a species $k$ schematically plotted as a function of $Y_c = (Y_{CO} + Y_{CO2}) - (Y_{CO} + Y_{CO2})^n$. Illustration of the determination of $\delta$ (Equation 34) and $\delta'$ (Equation 35).

Major and radical species feature different types of sources and diffusion terms distributions in composition space distributions. The magnitude of the O$_2$ diffusion term is larger near the unburned side, which cannot be balanced by the small source term at the same location, while for radicals, the diffusion term near the unburned side vanishes (Figure 16). Indeed, for radical species, the reaction zone and the diffusion zone extend approximatively over the same range; then a scaling relation reflecting the characteristic width of the reaction zone also reflects that of the diffusion zone. On the contrary, for a major species, since part of the diffusion zone is outside of the range of the reaction zone, a scaling relation based on the characteristic width of the reaction zone is not suitable to reflect the characteristic width of the whole diffusion zone. Due to the influence of the diffusion term, profiles of the reduced gradient $\partial Y_{k+}^+/\partial Y_{k,c}^+$ and of the reduced species mass fraction $Y_{k+}^+$ of O$_2$ depart from self-similarity and a different scaling is needed.

Figures 17 and 18 show information similar to Figures 15 and 16, but for set 3 of Table 2. The self-similar behavior of the diffusion term is improved. The slight discrepancies of source terms from self-similarity are cancelled out with those from the diffusion term. As a result, the reduced gradient $\partial Y_{k+}^+/\partial Y_{k,c}^+$ and the reduced species mass fraction $Y_{k+}^+$ exhibit excellent self-similar properties on the whole range of variation of $Y_{k,c}^+$. The impact of the scaling relation on the self-similarity expression of the major species and radicals can be explained further from Figure 19. As the dilution parameter changes, the ratio $\delta'/\delta$ (Equations 34 and 35) stays roughly constant for the CH radical, but decreases for the major species O$_2$. Therefore, the change of scaling relation from set 2 to set 3 has more effects on the self-similarity expression of O$_2$ than CH. This result has been retrieved for all major and radical species.

4.2. Self-similar response of adiabatic and non-adiabatic diluted flames

The self-similarity analysis has been applied to mass fractions and source terms of 10 species, including major (CH$_4$, O$_2$, CO$_2$, H$_2$O), minor (CO, H$_2$) and radical species (O, H, O$_2$, CO, H$_2$O, CO$_2$, H$_2$O).
Following the conclusions of the previous section, two different scaling relations are applied to achieve self-similarity for both mass fractions and source terms. For species mass fraction, transformations 2 or 3 of Table 2 are used; for species reaction rate, the progress variable $Y_c$ and species reaction rates are reduced with $Y_{k,c}$ defined in set 2 of Table 2.

The impact of burnt-gas dilution on self-similarity properties is first investigated. Figure 20 shows profiles of reduced species mass fractions and source terms for species CH$_4$, CO and OH, in the adiabatic cases (xix), (iv), (v) and (vi) of Table 1, where dilution varies from 0 to 0.24. Except for the source term of OH (Figure 20a), where a slight departure from self-similarity is observed, for all dilution levels a single curve is sufficient to describe the evolution of a given quantity (source term or mass fraction).

Varying the heat-loss parameter from zero to unity, self-similar properties are preserved. Figure 21 presents source terms and mass fraction responses for CH$_4$, H$_2$O and CH; the reference case (xix) without heat-loss is also shown for comparison. Varying also the equivalence ratio, the self-similar character is slightly altered, as summarized in Table 3. For most stoichiometric and lean flames, self-similarity is obtained; a departure is however observed for rich flames.

The reduced energy source term is plotted in Figure 22(a) for the 20 cases studied. A close-to-perfect self-similar property is obtained. Because the energy source term is a combination of all species sources, it may be concluded that self-similar properties mostly dominate for heat sensitive species. Some major species, such as O$_2$ (Figure 22b), exhibit a quasi-perfect self-similar response; others, such as H$_2$ and CO, are self-similar for lean and rich cases.

Figure 15. CH self-similarity based on set 2 of Table 2, $\phi = 1.0$. Solid line: case (iv); dot line: case (v); dash line: case (vi).
stoichiometric mixtures, but not for rich mixtures. This is illustrated in Figure 23; hopefully in premixed combustion systems, rich combustion is overall avoided.

### 4.3. Database reduction with self-similar properties

Various options exist to couple chemical lookup tables with flow solvers; they depend on numerous practical constraints, leading to different modeling approaches. In all cases, a

<table>
<thead>
<tr>
<th>Species</th>
<th>Source term</th>
<th>Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>LSR</td>
<td>LSR</td>
</tr>
<tr>
<td>O₂</td>
<td>LSR</td>
<td>LSR</td>
</tr>
<tr>
<td>CO₂</td>
<td>LSR</td>
<td>NS</td>
</tr>
<tr>
<td>H₂O</td>
<td>LSR</td>
<td>LSR</td>
</tr>
<tr>
<td>CO</td>
<td>LS</td>
<td>LS</td>
</tr>
<tr>
<td>H₂</td>
<td>LS</td>
<td>LS</td>
</tr>
<tr>
<td>O</td>
<td>LS</td>
<td>LS</td>
</tr>
<tr>
<td>H</td>
<td>LS</td>
<td>LSR</td>
</tr>
<tr>
<td>OH</td>
<td>LS</td>
<td>LSR</td>
</tr>
<tr>
<td>CH</td>
<td>LS</td>
<td>LSR</td>
</tr>
</tbody>
</table>
balance equation must be solved for $Y_c$, therefore its source $\dot{\omega}_c$ must be available. For $Y_k$, the species mass fractions, they can be transported with the flow and $\dot{\omega}_k$ must be tabulated, or the species vector can be read directly from the table [18, 20]. For energy transport, the energy source $\dot{\omega}_e$ can be tabulated directly or reconstructed from species sources.

From the self-similarity analysis conducted above, the estimation of $\dot{\omega}_k$ relies on two types of information:

1. The reduced reaction rate $\dot{\omega}_k^+(Y_{k,c}^+)$, expressed as a function of the reduced mass fraction $Y_{k,c}^+$. For most species discussed above, a single curve is sufficient to capture the whole range of equivalence ratio variation, dilution by burnt gases and heat-loss; this is done over $N_c$ points.

2. Scaling relations providing $Y_{k,c}^1$, $Y_{k,c}^2$ and $|\dot{\omega}_k^+|_{\text{max}}$ as functions of the equivalence ratio $\phi$, dilution rate $\alpha$, heat-loss factor $\beta$, initial pressure $P_0$ and initial fresh fuel–air mixture temperature $T_0$. In the particular case of constant values of $P_0$ and $T_0$, this database contains $3N_\phi \times N_\alpha \times N_\beta$ data, where $N_\phi$, $N_\alpha$ and $N_\beta$ are the numbers of discretization points covering the equivalence ratio range, the dilution rate, and heat-loss factor, respectively. The reduction factor between the self-similar table and the full table is:

$$r_1 = \frac{N_c \times N_\phi \times N_\alpha \times N_\beta}{N_c + 3N_\phi \times N_\alpha \times N_\beta}.\quad (36)$$

The parameters $Y_{k,c}^1$, $Y_{k,c}^2$ and $|\dot{\omega}_k^+|_{\text{max}}$ feature almost linear responses versus the dilution rate whatever the heat-loss and the equivalence ratio, as illustrated in Figures 24(a) and
25(a). Thus $Y_{k,c}^1$ or $Y_{k,c}^2$ evolution may be approximated from their values at $\alpha = 0$ and their slope as functions of $\beta$ and $\phi$. The maximum of the source term (Figures 24b and 22b) has a very smooth evolution and can be expressed as a second degree polynomial fit, implying the storage of three values for each $\phi$ and $\beta$. The reduction factor is then:

$$r_2 = \frac{N_c \times N_\phi \times N_\alpha \times N_\beta}{N_c + (2 \times 2 + 3)N_\phi \times N_\beta}.$$  

Typically for a table discretized over 100 points in every direction, $r_1 = 33$ and $r_2 = 1109$. Moreover, accessing the database is also much faster, as the four-dimensional lookup table is now replaced by seven two-dimensional data sets and one one-dimensional vector.

A similar analysis is conducted for tabulating species mass fractions. As for the source term, two types of information are needed:

1. The reduced mass fraction $Y_{k,c}^\pm (Y_{k,c,e})$ versus $Y_{k,c,e}$, with a single quasi-generic response valid for equivalence ratio variations, dilution by burnt gases and heat-loss.

2. Scaling relations providing $Y_{k,c}^1$, $Y_{k,c}^2$, $Y_{k,c}^{\max}$ and $Y_{k,c}^{\min}$ as functions of the table parameters; the reduction factor is then $r_1$. Figures 26 and 27 show the distribution of these quantities. They behave linearly versus the dilution, and $Y_{k,c}^1$ does not vary with heat-loss. $Y_{k,c}^{\min}$ (not plotted) stays close to zero for all minor and radical species and is a function of
Figure 19. Ratio $\delta/\delta'$ for species $O_2$ and $CH$, $\phi = 1.0$. Square: $O_2$; circle: $CH$.

Figure 20. Self-similar profiles of species reaction rate (top) and mass fraction (bottom) for adiabatic diluted premixed flames. (a),(d): $CH_4$; (b),(e): $CO$; (c),(f): $OH$. Solid: case (xix); dot: case (iv); dash: case (v); dot dash: case (vi).
Figure 21. Self-similar profiles of species reaction rate (top) and mass fraction (bottom) for adiabatic and non-adiabatic diluted premixed flames. (a),(d): CH$_4$; (b),(e): H$_2$O; (c),(f), CH. Solid: case (xix); dot: case (xiii); dash: case (xiv); dot dash: case (xv).

the equivalence ratio only for major species. The reduction table factor then reads:

$$r_3 = \frac{N_c \times N_\phi \times N_\alpha \times N_\beta}{N_c + 2 \times 2 \times N_\phi \times N_\beta + (2 + 1) \times N_\phi}.$$  \hspace{1cm} (38)

For 100 points in every direction, a reduction of 2475 is obtained.

Figure 22. Self-similar profiles of reaction rate and mass fraction. (a): $\dot{\omega}_\alpha$; (b): $Y_{\alpha2}$. Solid: $\phi = 1.0$; dot: $\phi = 0.7$; dash: $\phi = 1.4$. 
5. Coupling with flow solvers

The application of this type of chemistry tabulation to turbulent flames was already reported in [18, 20, 29, 30], without introducing self-similarity reduction. Other very similar approaches make use of flamelets as a sub-model for chemistry tabulation in turbulent flames [14, 31, 32]. The table is usually averaged or filtered using presumed probability density functions (pdf), to account for unresolved fluctuations of mixture fraction (equivalence ratio) and progress of the reaction; it was discussed in [28] how self-similarity observed in laminar flames is preserved by the averaging (RANS) or filtering (LES) operations. In the present work, only premixed flames are considered and the equivalence ratio is thus a fixed parameter. Two additional dimensions are added to the problem: the dilution rate, and the heat-loss in burnt gases, parameterized by $\alpha$ and $\beta$, respectively. In [22], heat-loss was added, neglecting unresolved fluctuations of enthalpy; this option may be retained in furnaces or boilers where large volumes of burnt gases associated with large residence times are found.

Figure 24. CH$_4$ scaling reaction rate, $\phi = 1.0$. Solid: $\beta = 0.0$; Dot: $\beta = 0.5$; dash: $\beta = 1.0$. (a) $|\dot{\omega}_k^{\max}|$, (b) solid: $Y_k^1$, bold: $Y_k^2$. 
Figure 25. CO scaling reaction rate, $\phi = 1.0$. Solid: $\beta = 0.0$; dot: $\beta = 0.5$; dash: $\beta = 1.0$. (a) $|\dot{\omega}_k^\text{max}|$, (b) solid: $Y_{k,c}^1$, bold: $Y_{k,c}^2$.

The chemical database that consists of species mass fractions, chemical rates, heat capacities and any other useful quantities is organized as:

$$\varphi_i = \varphi_i^\text{TAB}(c; \alpha, \beta)$$  (39)

where the equivalence ratio $\phi$ is omitted since it is assumed fixed in the following. $c$ is a reaction progress variable defined as $c = Y_c/Y_c^\text{Eq}(\alpha, \beta)$. In this formalism, for $c = 1$ various species concentrations are found in the products (Equation 39), depending on their temperature driven by vitiation by burnt gases ($\alpha$) and heat-loss ($\beta$). Once formed ($c \approx 1$), products can thus still evolve if the enthalpy ($\beta$) is non-uniform because of heat-loss.

The coupling procedure is first discussed assuming full resolution of the flow scales, as it would be done in DNS (Direct Numerical Simulation) performed with tabulated chemistry. The balance equations for the enthalpy $H$ [33] and for $c$ are solved, so that the three-dimensional fields $H(x,t)$ and $c(x,t)$ are available. In the equation for $c$ [5], in addition to convection, diffusion and source, terms exist due to non-uniformity of the

Figure 26. CH$_4$ scaling reaction rate, $\phi = 1.0$, $\phi = 1.0$. Solid: $\beta = 0.0$; Dot: $\beta = 0.5$; dash: $\beta = 1.0$. (a) $Y_k^\text{max} - Y_k^\text{min}$, (b) solid: $Y_{k,c}^1$, bold: $Y_{k,c}^2$. 
normalizing factor $Y^c_{Eq}(\alpha, \beta)$; these may be neglected, since their range of variation will not be that large here (see [5] for an analysis of the full $c$-equation with arbitrary normalizing factors). The two parameters $H$ and $c$ transported by the flow must be related to $\alpha$ and $\beta$, so that $\dot{\omega}_c(c; \alpha, \beta)$, the source of progress of the reaction, is determined to advance $c$ in time, along with the species concentration vector and other useful quantities provided by the relation (39).

Two main classes of combustion systems with recirculating burnt products may be considered. The first are with a controlled mass flow rate of recycled burnt gases (as in a low pressure EGR circuit in engines or in boilers [34]), then products are re-injected upstream of the main reaction zones to be well mixed with reactants prior to combustion; therefore the value of $\alpha$ is fixed (see Figure 1). In those systems, where the flame itself is almost adiabatic, $T_p$, the temperature of the re-injected burnt gases, after heat-loss in the recycling circuit is known, and thus $\beta$ from Equation (7).

The second are systems with products recirculating in large and coherent flow structures, as observed in the corners of combustion chambers [34, 35]. Away from the main turbulent flame, these recirculating burnt gases are partially mixed with fresh reactants, before entering the reaction zones; hence $\alpha(x,t)$ is non-uniform in space and time. The enthalpy is also non-uniform and so is $\beta(x,t)$; let us assume that this is mainly because of wall heat-transfer. However, before mixing with fresh fuel premixed with air, the burnt gases have a temperature $T_p^\star(t)$ that is usually not far from being locally uniform in space, at least in the vicinity of the fresh-gas injection [34]; this temperature close to fuel injection may be the lowest temperature taken by the products. In any case, this is known in the simulation from the temperature field, and $T_p^\star(t)$ may vary with time. The solving of the enthalpy balance equation, with proper boundary conditions to account for heat-loss at walls, then allows for determining $\alpha(x,t)$, the dilution rate distribution upstream of the reaction zone. According to Equation (4):

$$\alpha(x,t) = \frac{H(x,t) - H_f(T_f)}{H_p(T_p^\star(t)) - H_f(T_f)}.$$  (40)

It is clearly assumed in this formulation that dilution by burnt gases occurs upstream of the reaction zone.
The local value of $\beta$ must be selected so that the tabulated flamelet matches the local flow enthalpy. Once $\alpha(x, t)$ is know from Equation (40), one may write from Equations (7) and (4):

$$
\beta(x, t) = \frac{H(x, t) - H^f(T^f)}{\alpha(x, t)\left(H^p(T^f) - H^f(T^f)\right)}.
$$

(41)

In flames transferring heat at walls at $c = 1$, the chemical equilibrium composition evolves according to local enthalpy levels, as given by the burnt-gas flamelet composition for the proper enthalpy level. The above relations ensure that this composition is reached from the tabulation.

Extension to RANS or LES is straightforward from previous work [18, 20, 29, 30, 32], where similar databases were combined with presumed probability density functions for $\alpha = \beta = 0$. In a first approach, unresolved fluctuations of $\alpha$ and $\beta$ may be neglected. Pursuing such an averaging technique, an averaged or filtered table would read:

$$
\tilde{\phi}_i(x, t) = \tilde{\phi}_{i,\text{TAB}}(\tilde{c}(x, t), C(x, t); \alpha(x, t), \beta(x, t))
$$

(42)

where $\tilde{\cdot}$ denotes a favre averaged quantity; and $S_c$ is the unmixedness or normalized unresolved level of fluctuation of $c$ obtained from a balance equation for the unresolved $c$-variance [36]. This is a sound first step, since most of the actual numerical flame modeling using premixed flamelet tabulated chemistry is based on $\alpha = \beta = 0$; introducing non-zero values of these parameters would already be an improvement.

6. Summary

Reducing the chemical lookup table size is of premier importance in massively parallel computations, where this table needs to be stored on every processor – specifically when the number of degrees of freedom of the table increases because of additional dimensions, such as heat-loss at walls or through radiative transport and dilution by recirculating products. Premixed flamelets are basic ingredients of various models for premixed turbulent combustion and have been used to build such chemical lookup table.

For a given detailed chemical scheme, the response of one-dimensional unstrained and laminar flamelets to dilution of its reactants by products at various enthalpy levels has been examined in the light of potential self-similar behavior.

Instead of the usual physical space analysis, the self-similar formalism is studied in composition space, following a term-by-term approach, hence looking at the self-similar response of molecular diffusion and chemical source separately.

Three sets of reduced coordinates are discussed, leading to increasing levels of accuracy in the self-similar response. For both major and minor species, it is found that using self-similar expressions can greatly reduce the size of a chemical database constructed from canonical laminar flames. However, different scaling relations should be used when dealing with major and radical.

Formally, this is applicable to flamelet based chemistry tabulation grounded on one-dimensional unstrained and laminar premixed flames, more or less diluted with their adiabatic or non-adiabatic products; the application to different mixtures and flow conditions would required further study.
Acknowledgments

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References