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CRS4-CCT

Transport equations for an incompressible reactive flow with two separated phases.

VERSION 1.6

July 9, 2003

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Abstract

This report is devoted to the analysis of the premixed combustion modeling in the approximation leading to the sole use of a progress variable to characterize the mixture state. First, we shortly describe the TFC model to set the problematic. Then we recall the constitutive instantaneous equations and their averaged counterparts. We examine in details the limit case in which the reaction takes place in an infinitely thin sheet. This situation is formaly identical to the modelling of two separated fluids exchanging matter through their interface. In this case, their is an exact dependence of the so-called counter-gradient transport term on the source term. The form of the dependence proves the couter-gradient nature of the term which was up to now only intuited. It also shows that their is fundamentaly only one unclosed term in the averaged progress variable equation. We examine the closure assumption of the source term in this framework and naturally re-derive the TFC model. We propose the basic idea for a slight improvement of the TFC model that takes into account the finite speed of the increasing brush width. The treatment of the limit case is done by use of generalized functions. They are quite delicate to manipulate and their is no strong familiarity with them in the combustion modelling community leading to the effective difficulty in judging the correctness of the results. For this reason, we re-derive the corresponding results in the general case of regular functions.

Contents

1 Introduction

The Turbulent Flame Closure (TFC) model [1] requires the use of a transport equation for the progress variable c giving the state of progress, normalised between 0 and 1, of the combustion process. The unclosed equation for the progress variable reads:

$$\partial_t(\overline{\rho}\tilde{c}) + \nabla.(\overline{\rho}\tilde{u}\tilde{c}) = -\nabla.(\overline{\rho}\widetilde{u''c''}) + \overline{\rho}\tilde{\dot{\omega}}, \quad (1)$$

where ρ is the gas density, t is the time and u is the velocity. The term $\overline{\rho}\widetilde{u''c''}$ is the progress variable turbulent transport and $\overline{\rho}\tilde{\dot{\omega}}$ is the chemical source term.

Both Reynolds averages (denoted by over-line) and Favre averages (denoted by tilde) such as $\overline{\rho}\tilde{c}$ are used, with $c" = (c - \tilde{c})$. For the flamelets mechanism of premixed combustion, we assume that $P_u + P_b = 1$ as $P_i << 1$, where P_u, P_b and P_i are the probabilities of unburned mixture, combustion products and intermediate compositions. In this case the average density and the progress variable have the form $\overline{\rho} = \rho_u P_u + \rho_b P_b$, and $\tilde{c} = (\rho_b/\overline{\rho})P_b$. It is fundamentally more correct and a general practice to use an equation in terms of $\tilde{c}$, the Favre averaged progress variable, instead of the probability P_b. Physical meaning of $\tilde{c}$ is quite clear. It is in fact the coefficient of combustion completeness: $\tilde{c} = 0$ refers to reactants, it increases across the flame (inside premixed flame $0 < \tilde{c} < 1$) and $\tilde{c} = 1$ refers to products.

The closed equation coming from the TFC model is as follows:

$$\partial_t(\overline{\rho}\tilde{c}) + \nabla.(\overline{\rho}\tilde{u}\tilde{c}) = \nabla.(\overline{\rho}D_t\nabla\tilde{c}) + (\rho_u U_t)|\nabla\tilde{c}|, \quad (2)$$

For the motivation of such a closure, see for example [2] and its references. Here, we want to show that in the limit case of fast chemistry where the c function degenerates into the characteristic function of the burned phase, then the mean transport equation of $\tilde{c}$ can be derived analytically with only one term requiring a closure assumption. We also derive in a precise way the correct expression of the transport term of the momentum equation. This term is closed in the direction of $\nabla\tilde{c}$, but a closure assumption is still required in the directions parallel to the iso-surfaces of $\tilde{c}$.

2 System of equations

2.1 Instantaneous equations

We consider the following set of instantaneous equations.

Mass conservation:

$$\partial_t\rho + \nabla\cdot(\rho u) = 0, \quad (3)$$

Progress variable equation:

$$\partial_t c + u \cdot \nabla c \quad = \quad \frac{\dot{S}}{\rho}, \tag{4}$$

this form becomes undefined if u is discontinuous where c is also discontinuous, so we add the continuity equation to get a conservative form which circumnavigates this problem:

$$\partial_t(\rho c) + \nabla \cdot (\rho u c) \quad = \quad \dot{S}. \tag{5}$$

The simplest possibility for the source term $\dot{S}$ is:

$$\dot{S} \quad = \quad \rho_\star U_f |\nabla c|, \tag{6}$$

describing a variable mass consumption velocity rate such that the velocity variations due to the density variations are exactly compensated to keep unchanged the profile of c ($\rho_\star$ is a constant). The meaning of U_f changes according to the value taken by $\rho_\star$.

Momentum equation:

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P - \nabla \cdot \mu \nabla u \quad = \quad 0. \tag{7}$$

2.2 Averaged equations

The averaging of the former set leads to the following equations.

Mass conservation:

$$\partial_t \overline{\rho} + \nabla \cdot (\overline{\rho} \tilde{u}) \quad = \quad 0, \tag{8}$$

Progress variable equation:

$$\partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) \quad = \quad \overline{\dot{S}} + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) - \nabla \cdot \overline{\rho u c} \tag{9}$$

The simplest possibility for the source term $\overline{\dot{S}}$ is:

$$\overline{\dot{S}} \quad = \quad \rho_\star U_f \cdot \frac{\Sigma}{\Sigma_0} |\nabla \overline{c}|, \tag{10}$$

or in term of the Favre averaging:

$$\overline{\dot{S}} \quad = \quad \rho_\star U_f \cdot \frac{\Sigma}{\Sigma_0} \frac{\overline{\rho}^2}{\rho_u \rho_b} |\nabla \tilde{c}|, \tag{11}$$

where $\frac{\Sigma}{\Sigma_0}$ is a geometrical multiplier of the interface length over the minimum (straight) interface length.

We will see that the introduction of this expression in the progress variable equation for the bi-modal case leads to the same equation as for the TFC model but without diffusion term. This means that the diffusion term is a property of the source term, or in other words a property of the interface dynamics. This also means that this modelling assumption is insufficient.

Momentum equation:

$$\partial_t(\overline{\rho}\tilde{u}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{u}) + \nabla \overline{P} - \nabla \cdot \overline{\mu} \nabla \tilde{u} \quad = \quad \nabla \cdot (\overline{\rho}\tilde{u}\tilde{u}) - \nabla \cdot \overline{\rho u u}. \tag{12}$$

3 Derivations for the bimodal incompressible case

We consider the limit case of infinite fast chemistry where the progress variable can be only either zero or one and therefore coincide with the characteristic function of the burned side. We also consider that either the unburned and the burned sides are incompressible.

3.1 Additional equations

In the bimodal approximation of the combustion, the flow is composed of the juxtaposition of two incompressible flows, one is the unburned or fresh mixture (subscript u), the other is the products or burned mixture (subscript b). The region where lies the mixtures is defined by the value of a scalar, named c with value zero for the fresh mixture and one for the products. The variable c is some kind of limiting case of the classical progress variable. We express hereafter these concept in mathematical form. The problem is that the variables u_b and u_u (but also the constant ρ_b and ρ_u) have no physical meaning respectively in the unburnt and burnt region. But, because we want to write formula valid in all the domain considered we must extend u_b and u_u to the whole domain. The extension can be arbitrary but we want to be authorised to use the standard derivation rules like $\nabla \cdot (u_b c) = u_b \cdot \nabla c + c \nabla \cdot u$ taking into account that c is a discontinuous function. For this reason, we choose to consider regular extensions of u_b and u_u, preserving at least their continuity and the continuity of their divergence. Similarly, ρ_b and ρ_u are extended to a constant value all over the domain. Note that we can not extend the divergence free property of u_b and u_u to the entire domain when the interface has closed contours, but we will not need it. Nevertheless, by continuity, u_b and u_u are divergence free also on the interface. This property was already evidenced in [].

In mathematical form, it can be expressed as:

$$c \nabla \cdot u_b = 0 \tag{13}$$

$$(1-c) \nabla \cdot u_u = 0 \tag{14}$$

Density, pressure, velocity and momentum:

$$\rho = c\rho_b + (1-c)\rho_u \tag{15}$$

$$P = cP_b + (1-c)P_u \tag{16}$$

$$u = cu_b + (1-c)u_u \tag{17}$$

$$\rho u = c\rho_b u_b + (1-c)\rho_u u_u \tag{18}$$

$$\rho uu = c\rho_b u_b u_b + (1-c)\rho_u u_u u_u \tag{19}$$

Note that while these first two equations are in fact definitions, the three others are properties. Specifically u is the velocity associated to ρ.

These definitions lead to additional properties that can prove useful for the derivation of the unclosed terms. For example:

$$\begin{aligned}
\rho c &= c\rho_b & (20)\\
\rho uc &= c\rho_b u_b & (21)\\
c &= c^2 & (22)\\
c(1-c) &= 0 & (23)
\end{aligned}$$

and some mean variable properties ($\overline{u}_b$ and $\overline{u}_u$ are conditional averaging):

$$\begin{aligned}
\overline{\rho} &= (\frac{\tilde{c}}{\rho_b} + \frac{1-\tilde{c}}{\rho_u})^{-1} & (24)\\
\tilde{c} &= (\frac{1}{\overline{\rho}} - \frac{1}{\rho_u})(\frac{1}{\rho_b} - \frac{1}{\rho_u}) & (25)\\
\overline{\rho} &= \overline{c}\rho_b + (1-\overline{c})\rho_u & (26)\\
\overline{\rho}\tilde{c} &= \rho_b\overline{c} & (27)\\
\overline{\rho}(1-\tilde{c}) &= \rho_u(1-\overline{c}) & (28)\\
\overline{\rho u} &= \overline{c}\rho_b\overline{u}_b + (1-\overline{c})\rho_u\overline{u}_u & (29)\\
\tilde{u} &= \tilde{c}\overline{u}_b + (1-\tilde{c})\overline{u}_u & (30)\\
\tilde{u} &= \overline{u}_b - (1-\tilde{c})(\overline{u}_b - \overline{u}_u) & (31)\\
\tilde{u} &= \overline{u}_u + \tilde{c}(\overline{u}_b - \overline{u}_u) & (32)\\
\overline{u} &= \overline{\rho}(\frac{\tilde{c}\overline{u}_b}{\rho_b} + \frac{(1-\tilde{c})\overline{u}_u}{\rho_u}) & (33)\\
&= \tilde{u} + \overline{\rho}(\frac{1}{\rho_b} - \frac{1}{\rho_u})\tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u) & (34)\\
\overline{\rho uu} &= \overline{c}\rho_b\overline{u_b u_b} + (1-\overline{c})\rho_u\overline{u_u u_u} & (35)\\
\overline{\rho uc} &= \overline{c}\rho_b\overline{u_b} & (36)
\end{aligned}$$

We add some properties specific of the incompressibility, with eventual uncertainty linked to the variables value at the interface avoided thanks to our prolongation choice for u_b and u_u:

$$\begin{aligned}
\nabla\cdot\overline{u}_b &= 0 & (37)\\
\nabla\cdot\overline{u}_u &= 0 & (38)\\
\nabla\cdot\tilde{u} &= (\overline{u}_b - \overline{u}_u)\cdot\nabla\tilde{c} \text{ (from 31)} & (39)
\end{aligned}$$

3.2 Unclosed expression

Scalar transport (see formula in appendix):

$$\overline{\rho uc} = \rho_b \overline{u}_b \overline{c} \quad (40)$$

$$= \overline{\rho}\tilde{c}\overline{u}_b \quad (41)$$

$$= \overline{\rho}\tilde{c}[\tilde{u} + (1-\tilde{c})(\overline{u}_b - \overline{u}_u)] \quad (42)$$

$$\overline{\rho uc} = \overline{\rho}\tilde{c}\tilde{u} + \overline{\rho}\tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u) \quad (43)$$

Momentum transport:

$$\overline{\rho uu} = \overline{c}\rho_b \overline{u_b u_b} + (1-\overline{c})\rho_u \overline{u_u u_u} \quad (44)$$

$$\overline{u_b u_b} = \overline{u}_b \overline{u}_b + Dt_b \quad (45)$$

$$\overline{u_u u_u} = \overline{u}_u \overline{u}_u + Dt_u \quad (46)$$

$$\overline{\rho Dt} = \overline{c}\rho_b Dt_b + (1-\overline{c})\rho_u Dt_u \quad (47)$$

$$\overline{\rho uu} = \overline{c}\rho_b \overline{u}_b \overline{u}_b + (1-\overline{c})\rho_u \overline{u}_u \overline{u}_u + \overline{\rho Dt} \quad (48)$$

$$= \overline{\rho}\tilde{c}\overline{u}_b \overline{u}_b + \overline{\rho}(1-\tilde{c})\overline{u}_u \overline{u}_u + \overline{\rho Dt} \quad (49)$$

Noting that:

$$\tilde{u}\tilde{u} = [\overline{u}_b - (1-\tilde{c})(\overline{u}_b - \overline{u}_u)][\overline{u}_u + \tilde{c}(\overline{u}_b - \overline{u}_u)] \quad (50)$$

$$= \tilde{c}\overline{u}_b \overline{u}_b + (1-\tilde{c})\overline{u}_u \overline{u}_u - \tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u)(\overline{u}_b - \overline{u}_u) \quad (51)$$

it comes:

$$\overline{\rho uu} = \overline{\rho}\tilde{u}\tilde{u} + \overline{\rho}\tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u)(\overline{u}_b - \overline{u}_u) + \overline{\rho Dt} \quad (52)$$

3.3 Closed expression

We do not need to know the previous fluxes but only their divergence. The problem is to eliminate the terms using the un-resolved variable $\overline{u_b} - \overline{u_u}$. The method is to use the strong dependence of the progress variable equation and mass conservation equation. Starting from this later one (equation 8), we have:

$$\partial_t \overline{\rho} + \tilde{u} \cdot \nabla \overline{\rho} = -\overline{\rho} \nabla \cdot \tilde{u}. \quad (53)$$

we use that $\overline{\rho}$ is function of $\tilde{c}$ to express the LHS in terms of $\tilde{c}$:

$$\partial_{\tilde{c}} \overline{\rho} (\partial_t(\tilde{c}) + \tilde{u} \cdot \nabla \tilde{c}) = -\overline{\rho} \nabla \cdot \tilde{u}, \quad (54)$$

Multiplying by $\overline{\rho}$ and re-using the continuity equation, we have:

$$\partial_{\tilde{c}} \overline{\rho} [\partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c})] = -\overline{\rho}^2 \nabla \cdot \tilde{u}, \quad (55)$$

and using the expression of $\nabla \cdot \tilde{u}$, we get:

$$\partial_{\tilde{c}}\overline{\rho}[\partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c})] = -\overline{\rho}^2(\overline{u}_b - \overline{u}_u) \cdot \nabla\tilde{c}. \quad (56)$$

On another hand, using the progress variable equation 9 and equation 43, we have:

$$\partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) = \overline{\dot{S}} - \nabla \cdot [\overline{\rho}\tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u)] \quad (57)$$

and using the incompressibility of $\overline{u}_b - \overline{u}_u$:

$$\begin{aligned} \partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) &= \overline{\dot{S}} - (\overline{u}_b - \overline{u}_u) \cdot \nabla[\overline{\rho}\tilde{c}(1-\tilde{c})] \quad (58)\\ \partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) &= \overline{\dot{S}} - \partial_{\tilde{c}}[\overline{\rho}\tilde{c}(1-\tilde{c})](\overline{u}_b - \overline{u}_u) \cdot \nabla\tilde{c} \quad (59) \end{aligned}$$

Equations 56 and 59 form a system of two equations in the unknown $\partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c})$ and $(\overline{u}_b - \overline{u}_u) \cdot \nabla\tilde{c}$ which solution is:

$$\begin{aligned} \partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) &= \overline{\rho}^2\{\overline{\rho}^2 - \partial_{\tilde{c}}\overline{\rho} \cdot \partial_{\tilde{c}}[\overline{\rho}\tilde{c}(1-\tilde{c})]\}^{-1}\overline{\dot{S}} \quad (60)\\ (\overline{u}_b - \overline{u}_u) \cdot \nabla\tilde{c} &= \{\overline{\rho}^2 - \partial_{\tilde{c}}\overline{\rho} \cdot \partial_{\tilde{c}}[\overline{\rho}\tilde{c}(1-\tilde{c})]\}^{-1}\partial_{\tilde{c}}\overline{\rho} \cdot \overline{\dot{S}} \quad (61) \end{aligned}$$

Expanding the derivatives, calculation finally gives:

$$\begin{aligned} \partial_t(\overline{\rho}\tilde{c}) + \nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) &= \frac{\rho_b\rho_u}{\overline{\rho}^2}\overline{\dot{S}} \quad (62)\\ (\overline{u}_b - \overline{u}_u) \cdot \nabla\tilde{c} &= \frac{\rho_u - \rho_b}{\overline{\rho}^2}\overline{\dot{S}} \quad (63) \end{aligned}$$

The term $\nabla \cdot (\overline{\rho u c} - \overline{\rho}\tilde{u}\tilde{c})$ which was expected to have a counter-gradient nature [2] can be now described in term of the mean (positive) source term. It comes from 43 and 106:

$$\nabla \cdot (\overline{\rho}\tilde{u}\tilde{c}) - \overline{\rho u c}) = [\frac{\tilde{c}^2}{\rho_b} - \frac{(1-\tilde{c})^2}{\rho_u}](\rho_u - \rho_b)\overline{\dot{S}}. \quad (64)$$

This formula demonstrates the counter-gradient, or using an alternative terminology, the anti-diffusive nature of this term. In effect, it lowers the value of $\tilde{c}$ when $\tilde{c}$ is small and increases the value of $\tilde{c}$ when $\tilde{c}$ is close to one, thus sharpening the interface.

Momentum transport:

The momentum transport needs a closure assumption for the expression of $(\overline{u}_b - \overline{u}_u)$ in the directions parallel to the iso-surfaces of $\tilde{c}$ while it is already known in the direction of $\nabla\tilde{c}$. If we make the simplest assumption that $(\overline{u}_b - \overline{u}_u)$ and $\nabla\tilde{c}$ are parallel. That is:

$$(\overline{u}_b - \overline{u}_u) \wedge \nabla\tilde{c} = 0, \quad (65)$$

or equivalently

$$(\overline{u}_b - \overline{u}_u) \cdot \nabla \tilde{c} \quad = \quad -|\overline{u}_b - \overline{u}_u| \cdot |\nabla \tilde{c}|, \tag{66}$$

so that $\overline{\rho u u}$ is closed. This hypothesis looks very reasonable for the application in mind, at least where $\tilde{c}$ is not too close to zero or one. Under this assumption, we have:

$$\overline{u}_b - \overline{u}_u \quad = \quad -\frac{\rho_u - \rho_b}{\overline{\rho}^2}\overline{\dot{S}}\tilde{n} \tag{67}$$

where $\tilde{n} = \frac{-\nabla \tilde{c}}{|\nabla \tilde{c}|}$ and using equation 52 neglecting the diffusion term, it comes:

$$\overline{\rho u u} - \overline{\rho}\tilde{u}\tilde{u} \quad = \quad \frac{(\rho_u - \rho_b)^2}{\overline{\rho}^3}\tilde{c}(1-\tilde{c})\overline{\dot{S}}^2\tilde{n}\tilde{n}. \tag{68}$$

3.4 Closure of the progress variable equation source term

The analysis of the bimodal case leaves only one fundamentally unclosed term, the source term. The "turbulent transport" which is usually unclosed in a more general case result to be algebraically related to the closure of the unclosed source term, $\dot{S}$. It has already been seen that the "turbulent transport" is an anti-diffusive term $\nabla \cdot (\overline{\rho u c} - \overline{\rho}\tilde{u}\tilde{c})$ is an anti-diffusive term in our case and act as a multiplier by $\frac{\rho_b \rho_u}{\overline{\rho}^2}$ of $\overline{\dot{S}}$ so that the determination of $\overline{\dot{S}}$ completely closes the equation.

For the application foreseen (turbulent combustion with flame anchoraging), the main characteristic of the flame is an instantaneous strongly corrugated thin sheet included in an increasing brush width.

The representation of $\overline{\dot{S}}$ in the form $\rho_\star U_f \cdot \frac{\Sigma}{\Sigma_0}\frac{\overline{\rho}^2}{\rho_u \rho_b}|\nabla \tilde{c}|$ takes into account only the highly corrugated aspect of the instantaneous flame but not the increasing brush width. In this discussion, we will consider that each aspect can be considered separately and that $\overline{\dot{S}}$ is the sum of two contributions, the first one, $\overline{\dot{S}}_{tr}$, characterising the global flame speed by means of a standard transport term and the second, $\overline{\dot{S}}_{diff}$ characterising the increasing brush by means of a diffusing term.

$$\overline{\dot{S}} \quad = \quad \overline{\dot{S}}_{tr} + \overline{\dot{S}}_{diff}. \tag{69}$$

The modelling can now be reformulated as:

$$\overline{|\nabla c|} \quad = \quad \frac{\Sigma}{\Sigma_0}|\nabla \overline{c}| + \quad \text{diffusion effects}, \tag{70}$$

leading to:

$$\overline{\dot{S}}_{tr} \quad = \quad (\rho_\star U_f) \cdot \frac{\Sigma}{\Sigma_0}\frac{\overline{\rho}^2}{\rho_u \rho_b}|\nabla \tilde{c}|. \tag{71}$$

For the modelling of $\frac{\Sigma}{\Sigma_0}$, refer to the TFC model. Some improvement may be foreseen by giving a dependence of this term on $\tilde{c}$.

In the TFC model, the diffusive term is modelled as a standard turbulent diffusion term whose expression in frame of our derivation is:

$$\overline{\dot{S}}_{tr} = \frac{\overline{\rho}^2}{\rho_u \rho_b} \nabla \cdot (D_t \nabla \tilde{c}). \tag{72}$$

Once again, refer to the TFC model [1] for the expression of D_t.

This expression for $\overline{\dot{S}}_{tr}$ has to be considered as a rough approximation. In effect, being a second order term in space in a first order equation in time, it gives a parabolic nature to the equation. In other word, the diffusion takes place at infinite speed, which is largely exaggerated in this context where the diffusion should takes place at finite speed roughly proportional to the turbulent pulsation. To solve this problem, one has basically two solutions, both aimed at giving an hyperbolic character to the equation. The first one is to to keep the former diffusive term and add a term in the equation which is second order in time term. In fact, whemn the mean velocity is not zero, this method leads to the inclusion of several second order terms giving a much more complicated equation, not likely to be implemented in commercial CFD tools. The second method is to generate a first order in space diffusive term. The diffusive term may be of a form similar to:

$$\overline{\dot{S}}_{diff} = \frac{\overline{\rho}^2}{\rho_u \rho_b} (1 - 2\tilde{c})\ U_{diff} |\nabla \tilde{c}| \tag{73}$$

where U_{diff} is order the turbulent pulsation and coincide with the expansion velocity of the flame brush width.

4 Extension to the general case

The former results have been obtained in the limit case of infinitely fast chemistry where the progress variable takes only the values zero and one and has probability zero to have an intermediate value. The advantage is that a lot of relations are highly simplified. Mainly, the mean of the progress variable coincide with the probability of being in the burned gas. The drawbacks of this approach is that we are obliged to deal with generalised functions whose correct manipulation and understanding is quite delicate and not so widely widespread. One way to demonstrate that the former derivations have been done properly is to obtain the same result as the limit for thin flame of the general case, therefore manipulating only regular functions. The computation is much more difficult to infer in the general case, but as we know the final result (ie what to look for), we can quite artificially get right to it.

In the general case, we split the probability space in three complementary domains:

- P_b is the probability of being in the burned region where $c = 1$,
- P_u is the probability of being in the unburned region where $c = 0$,
- P_i is the probability of being in the intermediate region where $0 < c < 1$.

Indices b,u and i will refer respectively to the conditional probabilities of being in the burned, unburned and intermediate regions.

4.1 Formula in the general case

Because we consider an incompressible gas and the reaction is supposed to take place only inside the intermediary region, we have:

$$\nabla \cdot \overline{u}_b = 0, \tag{74}$$

$$\nabla \cdot \overline{u}_u = 0, \tag{75}$$

$$\overline{\rho}_b = \rho_b, \tag{76}$$

$$\overline{\rho}_u = \rho_u. \tag{77}$$

In the former derivations, we strongly used the fact that $\overline{\rho}$ and $\tilde{c}$ are linked through simple algebraic relations. As we will use these relations, they must keept true in the general case. This is obtain by requiring an affine relation between ρc and ρ, that is $\rho c = a\rho + b$ where a and b are constant. This leads to the following relation, in fact defining the progress variable c:

$$\rho = (\frac{c}{\rho_b} + \frac{1-c}{\rho_u})^{-1}, \tag{78}$$

leading to:

$$\overline{\rho} = (\frac{\tilde{c}}{\rho_b} + \frac{1-\tilde{c}}{\rho_u})^{-1}, \tag{79}$$

$$\tilde{c} = (\frac{1}{\overline{\rho}} - \frac{1}{\rho_u})(\frac{1}{\rho_b} - \frac{1}{\rho_u}). \tag{80}$$

The affine relation leads to:

$$\overline{\rho}\tilde{c} = (\frac{1}{\rho_b} - \frac{1}{\rho_u})^{-1}(1 - \frac{\overline{\rho}}{\rho_u}), \tag{81}$$

$$1 = (\frac{1}{\rho_b} - \frac{1}{\rho_u})\overline{\rho}\tilde{c} + \frac{\overline{\rho}}{\rho_u}, \tag{82}$$

$$\overline{\rho} = \rho_u - \frac{\rho_u - \rho_b}{\rho_b}\overline{\rho}\tilde{c}, \tag{83}$$

which are three formulations of the same property. As a consequence, the formula given in appendix are also valid in the general case.

We express the mean variables in terms of probability:

$$\overline{\rho} = \rho_b P_b + \rho_u P_u + \overline{\rho}_i P_i, \tag{84}$$
$$\overline{\rho c} = \rho_b P_b + \overline{\rho c}_i P_i, \tag{85}$$
$$\overline{\rho u} = \rho_b \overline{u}_b P_b + \rho_u \overline{u}_u P_u + \overline{\rho u}_i P_i, \tag{86}$$
$$\overline{\rho c u} = \rho_b \overline{u}_b P_b + \overline{\rho c u}_i P_i. \tag{87}$$

As the progress variable is between zero and one, the probabilities sum to one:

$$P_b + P_u + P_i = 1. \tag{88}$$

Making elementary substitutions in equations 85 to 87, we can express P_u and P_b in terms of the mean variables and P_i:

$$P_b = \frac{\overline{\rho c}}{\rho_b} - \frac{\overline{\rho c}_i}{\rho_b} P_i \tag{89}$$
$$P_u = \frac{\overline{\rho} - \overline{\rho c}}{\rho_u} - \frac{\overline{\rho}_i - \overline{\rho c}_i}{\rho_u} P_i. \tag{90}$$

4.2 Results in the general case

We are now able to generate the mean variables in a new usable form, by eliminating P_b and P_u from equation 85 to 87:

$$\overline{\rho u} = \overline{\rho c}\,\overline{u}_b - \overline{\rho c}_i P_i \overline{u}_b + \overline{\rho}\,\overline{u}_u - \overline{\rho c}\,\overline{u}_u + \overline{\rho}_i P_i \overline{u}_u - \overline{\rho c}_i P_i \overline{u}_u + \overline{\rho u}_i P_i \tag{91}$$
$$\overline{\rho u} = \overline{\rho}\tilde{c}(\overline{u}_b - \overline{u}_u) + \overline{\rho}\,\overline{u}_u + \varepsilon_1(P_i). \tag{92}$$

This gives a new expression for $\tilde{u}$:

$$\tilde{u} = \tilde{c}(\overline{u}_b - \overline{u}_u) + \overline{u}_u + \varepsilon_2(P_i) \tag{93}$$

and for $\nabla \cdot \tilde{u}$:

$$\nabla \cdot \tilde{u} = (\overline{u}_b - \overline{u}_u) \cdot \nabla \tilde{c} + \varepsilon_3(P_i), \tag{94}$$

which is the first expected result.

Now we deal with $\overline{\rho c u}$ and $\overline{\rho}\tilde{c}\tilde{u}$.

$$\overline{\rho c u} = \overline{\rho c}\,\overline{u}_b - \overline{\rho c}_i P_i \overline{u}_b + \overline{\rho c u}_i P_i, \tag{95}$$
$$\overline{\rho c u} = \overline{\rho}\tilde{c}\overline{u}_b + \varepsilon_4(P_i), \tag{96}$$

and

$$\overline{\rho c u} - \overline{\rho}\tilde{c}\tilde{u} = \overline{\rho}\tilde{c}\overline{u}_b - \overline{\rho}\tilde{c}[\tilde{c}(\overline{u}_b - \overline{u}_u) + \overline{u}_u] + \varepsilon_5(P_i) \tag{97}$$
$$\overline{\rho c u} - \overline{\rho}\tilde{c}\tilde{u} = \overline{\rho}\tilde{c}(1 - \tilde{c})(\overline{u}_b - \overline{u}_u) + \varepsilon_5(P_i), \tag{98}$$

which is the second expected result.

To model he source term, we have used a relation between the Favre and Reynolds average of the progress variable. So, we have to derive its counterpart in the general case.

$$\begin{aligned}
\overline{c} &= P_b + \overline{c}_i P_i && (99)\\
&= \frac{\overline{\rho c}}{\rho_b} - \frac{\overline{\rho c_i}}{\rho_b} P_i + \overline{c}_i P_i && (100)\\
\overline{c} &= \frac{\overline{\rho}\tilde{c}}{\rho_b} + \varepsilon_6(P_i). && (101)
\end{aligned}$$

All the results in the bimodal case are therefor valid in the general case up to a function of order P_i and letting P_i go to zero, we get back the results of the bimodal case.

5 Conclusion

Starting from the constitutive instantaneous equations and their averaged counterparts, we have examined in details the limit case in which the reaction takes place in an infinitely thin sheet. This situation is formaly identical to the modelling of two separated fluids exchanging matter through their interface. In this case, we have shown that their is an exact dependence of the so-called counter-gradient transport term on the source term. The form of the dependence proves the couter-gradient nature of the term which was up to now only intuited. It also shows that their is fundamentaly only one unclosed term in the averaged progress variable equation. We have examined the closure assumption of the source term in this framework and naturally re-derived the TFC model. We have proposed the basic idea for a slight improvement of the TFC model that takes into account the finite speed of the increasing brush width. These results have been extended to the general case, arriving to the same conclusion up to a term of order P_i, the probability to be inside the flamelet. The extension has been done without requiring the use of generalized functions.

A Additional formula

From the functional dependence of $\overline{\rho}$ on $\tilde{c}$, it comes:

$$\nabla\overline{\rho} = -(\frac{1}{\rho_b} - \frac{1}{\rho_u})\overline{\rho}^2\nabla\tilde{c} \tag{102}$$

$$\partial_t\overline{\rho} = -(\frac{1}{\rho_b} - \frac{1}{\rho_u})\overline{\rho}^2\partial_t\tilde{c} \tag{103}$$

$$\nabla(\overline{\rho}\tilde{c}) = -\frac{1}{\rho_u}(\frac{1}{\overline{\rho_b}} - \frac{1}{\overline{\rho_u}})^{-1}\nabla\overline{\rho} \tag{104}$$

$$= \frac{1}{\rho_u}\overline{\rho}^2\nabla\tilde{c} \tag{105}$$

$$\nabla[\overline{\rho}\tilde{c}(1-\tilde{c})] = -[\frac{\tilde{c}^2}{\rho_b} - \frac{(1-\tilde{c})^2}{\rho_u}]\overline{\rho}^2\nabla\tilde{c} \tag{106}$$

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