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A stable pressure-correction scheme for variable density flows involving non-premixed combustion

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SUMMARY

An efficient time-accurate algorithm is presented for numerical simulations of low-Mach number variable density flows in the context of non-premixed flames. The algorithm is based on a segregated solution formalism in the class of pressure-correction methods. It shows good conservation properties and returns stable results, regardless of the difference in density between neighboring cells. A simplified Burke–Schumann flame model is used to describe the heat release due to mixing of fuel and oxidizer. The convergence rate of the method is discussed for a 1D channel flow, containing fuel and oxidizer. Copyright © 2008 John Wiley & Sons, Ltd.

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KEY WORDS: low Mach; pressure correction; non-premixed combustion; conservation; stability

1. INTRODUCTION

With the introduction of large eddy simulation in turbulent combustion simulations, demanding time-accurate solutions, the generally applied pressure-correction schemes could no longer be used because of lack of stability. Recent literature on this topic is found in, e.g. [1–9]. Several authors [1–4] reported instability problems when the density ratio exceeds 4. The use of a predictor–corrector method [5] or a variable coefficient pressure equation [3] can stabilize the solution up to a higher density ratio but at the expense of loss of conservation properties [5] or with a modified state equation [6, 7]. In many combustion applications, higher density ratios regularly appear (e.g. for methane–air combustion, density ratios in the order of 10 near the flame front).

Previously [10], a pressure Poisson equation was determined for non-reacting variable density flows, whether a conduction or a mixing problem is considered. In none of these cases, a problem

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appeared, since $\partial\rho/\partial T$ or $\partial\rho/\partial\xi$ (T, temperature; ξ, species mass fraction) is uniquely defined and returns coefficients in the pressure Poisson equation that are constant in space. The situation in combustion problems is different, because of the non-linearity in the determination of the density field in terms of mixture fraction.

The purpose of the present study is to obtain a pressure-correction algorithm which (1) conserves total mass, (2) conserves fuel elements mass and (3) is stable and robust, without the need for any (unphysical) under-relaxation. It will become clear that conservation of both mass and fuel elements mass, together with the fulfillment of the equation of state, is impossible without iteration.

2. GOVERNING EQUATIONS

The basic equations are the Navier–Stokes equations for the flow field, with an additional equation, describing the mixing of fuel and oxidizer. The conservation of mass, momentum and fuel elements mass is then formulated as [11]

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u_i}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial\rho u_i}{\partial t}+\frac{\partial\rho u_i u_j}{\partial x_j}+\frac{\partial p_2}{\partial x_i}=\frac{\partial\tau_{ij}}{\partial x_j} \tag{2}$$

$$\frac{\partial\rho\xi}{\partial t}+\frac{\partial\rho\xi u_i}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\xi}{\partial x_i}\right) \tag{3}$$

In these equations, ρ denotes the density, u the velocity, p_2 the kinematic pressure, τ_{ij} the molecular viscous stress, ξ the mixture fraction and D the mass diffusion coefficient.

3. SIMPLIFIED EQUATION OF STATE FOR REACTING FLOW

For simplicity, a modified Flame-Sheet chemistry model is used. In the Flame-Sheet model, infinitely fast irreversible chemistry is assumed. This is a valid assumption when the chemical time scales are much smaller than the fluid-mechanical time scales. By this assumption, only one-step chemistry is considered, given by the reaction, involving fuel (F), oxidizer (O) and products (P): $v_F F+v_O O\rightleftharpoons v_P P$. If the reaction is also irreversible, it can proceed only from left to right. As a result, fuel and oxidizer cannot be found together at the same location. The resulting flamelet is called the Burke–Schumann flame structure. The mixture fraction is here defined as $\xi=(sY_F-Y_O+Y_O^0)/(sY_F^0+Y_O^0)$. Y_F^0 and Y_O^0 are fuel and oxidizer mass fractions in pure fuel and oxidizer streams, respectively, and $s=v_O W_O/v_F W_F$ is the stoichiometric ratio. The mixture fraction at stoichiometric conditions is then defined by $\xi_{\mathrm{st}}=Y_O^0/(sY_F^0+Y_O^0)$. The chemical properties are then given as a function of ξ,

$$\begin{aligned}
&Y_F(\xi)=Y_F^0\frac{\xi-\xi_{\mathrm{st}}}{1-\xi_{\mathrm{st}}},\quad Y_O(\xi)=0,\quad Y_P(\xi)=1-Y_F-Y_O\quad\text{for }\xi\leqslant\xi_{\mathrm{st}}\\
&Y_F(\xi)=0,\quad Y_O(\xi)=Y_O^0\frac{\xi_{\mathrm{st}}-\xi}{\xi_{\mathrm{st}}},\quad Y_P(\xi)=1-Y_F-Y_O\quad\text{for }\xi\geqslant\xi_{\mathrm{st}}
\end{aligned} \tag{4}$$

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The temperature is given as

$$\begin{aligned} T(\xi) &= \xi T_F^0 + (1-\xi)T_O^0 + \Delta T \frac{\xi}{\xi_{\mathrm{st}}} \quad \text{for } \xi \leqslant \xi_{\mathrm{st}} \\ T(\xi) &= \xi T_F^0 + (1-\xi)T_O^0 + \Delta T \frac{1-\xi}{1-\xi_{\mathrm{st}}} \quad \text{for } \xi \geqslant \xi_{\mathrm{st}} \end{aligned} \tag{5}$$

with $\Delta T = (q^0/c_p)\xi_{\mathrm{st}}$ and q^0 the heat release due to reaction. The above expressions can now be used to determine the density, $\rho(\xi) = (p_0/R)W(\xi)/T(\xi)$, with $W(\xi)$ the mean molecular weight, given by $1/W(\xi) = \sum_{i=1}^{N} Y_i(\xi)/W_i$. For the one-step chemistry, $\rho(\xi)$ reads

$$\begin{aligned} \rho(\xi) &= \frac{p_0}{R}\left[\frac{Y_O(\xi)}{W_O} + \frac{1-Y_O(\xi)}{W_P}\right]^{-1} \frac{1}{T(\xi)} \quad \text{for } \xi \leqslant \xi_{\mathrm{st}} \\ \rho(\xi) &= \frac{p_0}{R}\left[\frac{Y_F(\xi)}{W_F} + \frac{1-Y_F(\xi)}{W_P}\right]^{-1} \frac{1}{T(\xi)} \quad \text{for } \xi \geqslant \xi_{\mathrm{st}} \end{aligned} \tag{6}$$

This can be put under a short notation:

$$\rho(\xi) = \frac{p_0}{R} \frac{1}{a(\xi/\xi_{\mathrm{st}})^2 + b(\xi/\xi_{\mathrm{st}}) + c}$$

For the discussion of the algorithm, a further simplification is made: the quadratic term $(a(\xi/\xi_{\mathrm{st}})^2)$ in the denominator is zero, if we assume that all molecular weights W_F, W_O and W_P are the same. In that case, the change in density is only due to the release of heat in the reaction zone, not because of the reaction itself (through the formation of other species). We obtain formally

$$\rho(\xi) = \frac{p_0}{R} \frac{1}{b(\xi/\xi_{\mathrm{st}}) + c} \;\Leftrightarrow\; \rho = \frac{p_0}{cR} - \frac{b}{c\xi_{\mathrm{st}}}\rho\xi = \alpha\rho\xi + \beta \tag{7}$$

so that ρ is piecewise linearly dependent on $\rho\xi$. Expressions (7) are illustrated in Figure 1.

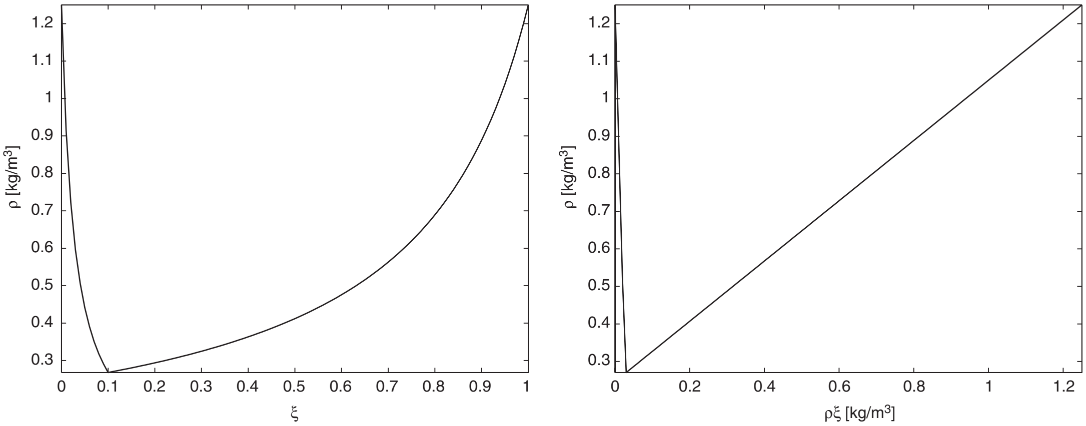

Figure 1. Density as a function of mixture fraction (ξ) and fuel mass ($\rho\xi$), if we assume all molecular weights to be equal and the same inlet temperature for fuel and oxidizer.

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4. GENERAL PRESSURE-CORRECTION FORMALISM

In the segregated solution procedure, a number of substeps are taken to determine the state at a next time level. Assuming we know the variables at time n, the state at time level $n+1$ is calculated as follows. First, the density at the new time is determined from the continuity equation. Doing so, mass is conserved. In a 1D discrete space, we obtain

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x}(\rho_R^n u_{i+1/2}^n - \rho_L^n u_{i-1/2}^n) \tag{8}$$

where the subscripts L and R refer to extrapolated values at the left and right face of the control volume. For a first-order upwind scheme, with positive values for the velocity, $\rho_L = \rho_{i-1}$, $\rho_R = \rho_i$. The velocity field is determined in two steps. First a prediction is made, using the momentum equations with the pressure term evaluated at time level n

$$(\rho u)_i^* = (\rho u)_i^n - \frac{\Delta t}{\Delta x}((\rho u)_R^n u_{i+1/2}^n - (\rho u)_L^n u_{i-1/2}^n) - \frac{\Delta t}{\Delta x}(p_{i+1/2}^n - p_{i-1/2}^n) + \Delta t \frac{\delta \tau^n}{\delta x} \tag{9}$$

The predicted field is corrected to give the velocity at the new time level, $(\rho u)_i^{n+1} = (\rho u)_i^* + (\rho u)_i'$ where the correction for the momentum $(\rho u)_i'$ is related to the correction for the pressure $p_i' = p_i^{n+1} - p_i^n$ by

$$\frac{(\rho u)_i'}{\Delta t} = -\frac{p_{i+1/2}' - p_{i-1/2}'}{\Delta x}$$

The correction for the pressure follows from inversion of an elliptic equation, based on a constraining equation for the velocity field.

5. ELEGANT ITERATIVE SCHEME FOR REACTING FLOWS

In order to fulfill all the requirements of stability and conservation, we reconsider the problem from a 1D discrete point of view. The following equations are important (with $f = \rho\xi$):

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} + \frac{\rho_R^n u_{i+1/2}^n - \rho_L^n u_{i-1/2}^n}{\Delta x} = 0 \tag{10}$$

$$\begin{aligned} &\frac{\rho_i^{n+1} u_i^{n+1} - \rho_i^n u_i^n}{\Delta t} + \frac{(\rho u)_R^n u_{i+1/2}^n - (\rho u)_L^n u_{i-1/2}^n}{\Delta x} \\ &\quad = -\frac{\rho_i^{n+1}}{2}\left[\frac{p_{i+1}^{n+1} - p_i^{n+1}}{\rho_{i+1/2}^{n+1}\Delta x} + \frac{p_i^{n+1} - p_{i-1}^{n+1}}{\rho_{i-1/2}^{n+1}\Delta x}\right] + \frac{\partial \tau_{ij}}{\partial x_j} \end{aligned} \tag{11}$$

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{f_R^n u_{i+1/2}^n - f_L^n u_{i-1/2}^n}{\Delta x} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial \xi}{\partial x_i}\right) \tag{12}$$

A constraint for u^{n+1} is found by combining (10) and (12), shifted at the next time level:

$$\frac{\rho_i^{n+2}-\rho_i^{n+1}}{\Delta t}+\frac{\rho_R^{n+1}u_{i+1/2}^{n+1}-\rho_L^{n+1}u_{i-1/2}^{n+1}}{\Delta x}=0 \tag{13}$$

$$\frac{f_i^{n+2}-f_i^{n+1}}{\Delta t}+\frac{f_R^{n+1}u_{i+1/2}^{n+1}-f_L^{n+1}u_{i-1/2}^{n+1}}{\Delta x}=\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial \xi}{\partial x_i}\right) \tag{14}$$

We define a chemical operator $\mathscr{H}_C$ as $\rho=\mathscr{H}_C(f)$. In case of pure mixing, the operator is purely linear. In case of combustion, however, this operator is highly non-linear. The constraint is now formulated by requiring $\rho^{n+2}=\mathscr{H}_C(f^{n+2})$, or

$$\begin{aligned}\rho_i^{n+1}-\Delta t\frac{\rho_R^{n+1}u_{i+1/2}^{n+1}-\rho_L^{n+1}u_{i-1/2}^{n+1}}{\Delta x}\\ =\mathscr{H}_C\left(f_i^{n+1}-\Delta t\frac{f_R^{n+1}u_{i+1/2}^{n+1}-f_L^{n+1}u_{i-1/2}^{n+1}}{\Delta x}+\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial \xi}{\partial x_i}\right)\right)\end{aligned} \tag{15}$$

Inserting $u^{n+1}=u^*+u'$, yields

$$\rho^*+\rho'=\mathscr{H}_C(f^*+f') \tag{16}$$

with

$$\rho^*=\rho_i^{n+1}-\Delta t\frac{\rho_R^{n+1}u_{i+1/2}^{*}-\rho_L^{n+1}u_{i-1/2}^{*}}{\Delta x}$$

$$f^*=f_i^{n+1}-\Delta t\frac{f_R^{n+1}u_{i+1/2}^{*}-f_L^{n+1}u_{i-1/2}^{*}}{\Delta x}+\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial \xi}{\partial x_i}\right)$$

$$\rho'=-\Delta t\frac{\rho_R^{n+1}u_{i+1/2}'-\rho_L^{n+1}u_{i-1/2}'}{\Delta x}$$

$$f'=-\Delta t\frac{f_R^{n+1}u_{i+1/2}'-f_L^{n+1}u_{i-1/2}'}{\Delta x}$$

Equation (16) can be linearized around f^*, resulting in

$$\rho^*+\rho'=\mathscr{H}_C(f^*)+\frac{\mathrm{d}\mathscr{H}_C}{\mathrm{d}f}(f^*)f' \tag{17}$$

Equation (17) can be expressed in system notation, with matrices A and B, pressure-correction vector $\mathbf{p}'$:

$$\left(A-\frac{\mathrm{d}\mathscr{H}_C}{\mathrm{d}f}(\mathbf{f}^*)B\right)\mathbf{p}'=\mathrm{RHS} \tag{18}$$

with RHS $=\mathscr{H}_C(\mathbf{f}^*)-\boldsymbol{\rho}^*$. The system is solvable at low cost if the matrices A and B do not change during iteration. Unfortunately, this is not true, since the matrices are composed of extrapolated values of density and fuel mass, which depend on the sign of the unknown velocity u^{n+1}. The same holds for the RHS, whose value also depends on the sign of u^{n+1}.

In order to save computing time, a minor assumption is introduced at this level: the extrapolated values for density and mixture fraction are calculated, based on the sign of u^*, instead of u^{n+1}. This assumption is not dramatic, since the evolution in time of the mixture fraction, where the sign of u^* is different from the sign of u^{n+1}, is mainly governed by diffusion ($(\partial/\partial x_i)(\rho D \partial\xi/\partial x_i)$ is the most important term in RHS) and not by convective transport. Because of the assumption, the mixture fraction does no longer remain bounded between 0 and 1. However, because of diffusion, the unboundedness is minimal. In order to obtain values for the mixture fraction between 0 and 1, a minimal amount of clipping is needed.

6. RESULTS AND DISCUSSION

The above pressure-correction scheme is validated on a 1D contact discontinuity. A 1D channel is filled with fuel on one side, and oxidizer on the other side. At the inlet a velocity of 1 m/s is imposed, so the velocity is 1 m/s in the entire domain. Diffusivity is set to zero ($D=0$). However, the effect of numerical diffusion due to the use of a first-order upwinding will affect the result. The initial conditions and the result after 10 time steps are shown in Figure 2. Ideally, the velocity field should be constant in the entire domain. However, because of numerical diffusion, a reaction zone is formed, resulting in a zone with lower density, and requiring the flow to accelerate towards the outlet. If the diffusion term is not set to zero, the result remains stable (not shown). It is, however, more important to look at the convergence of the elliptic equation. It is found that for this test case, with or without diffusion, mostly one, at most two iterations are needed in order to obtain density and mixture fraction fields that match according to the equation of state.

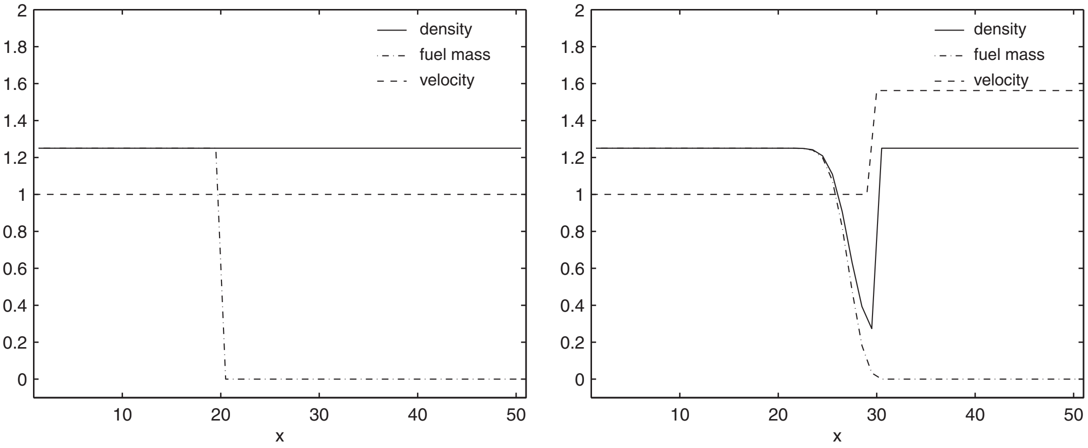

Figure 2. Density, fuel elements mass and velocity: initial field and state after 10 time steps.

7. CONCLUSION

We presented a new constraining equation for the determination of the elliptic equation for the pressure in pressure-correction methods. It conserves both mass and fuel elements mass, and obeys the equation of state. Furthermore, the algorithm remains stable, even for interfaces with sharp density ratios. The algorithm is validated on a combustion problem, using a simple flame-sheet chemistry model. It is reported that in that case, mostly only one iteration step for the pressure-correction is required. According to our experience, at most two iterations were encountered, making the pressure equation solvable at low cost and thus creating an efficient algorithm for time-accurate non-premixed combustion systems.

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