Numerical algorithms for premixed flames in closed channels*

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Abstract. An efficient numerical algorithm to study flame evolution in closed channels for low, but distinct from zero, Mach numbers is proposed. The system of Navier-Stokes equations for a compressible, chemically reacting gas mixture was considered as the mathematical model. Numerical algorithms are based on upwind finite-difference schemes of high order approximation and employ locally preconditioned iterations in order to obtain solution to the implicit system of grid equations on each time step.

1 Introduction

Slow combustion of premixed gases is characterised by the induced gas motion with speeds of order of normal flame front velocity $u_\text{f}$, which is much less than the speed of sound $c$. On the other hand, substantial heat release causes considerable expansion of gases undergoing exothermic chemical reaction. For example, combustion of air mixtures of hydrocarbon gases may decrease the gas density by a factor of four, see [Zeldovich (85)]. Thus, mathematical models of these phenomena should take compressibility into account.

The necessity to consider compressibility within the framework of the Navier-Stokes model raises the problem of compressible low Mach number flows. This problem can be effectively solved by using asymptotic expansions of solutions to the Navier-Stokes equations for a compressible fluid as the Mach number tends to zero [Rehm (78)]. Unfortunately, such an approach would neglect interaction of acoustic perturbations with the flame, which is possible at some stages of gas combustion in closed channels [Markstein (64)].

Really, besides the straightforward condition of validity of asymptotic expansions $M \ll 1$, there is an additional limitation on the applicability of the low Mach number model in flows with fast chemical reactions. It reads

$$M \ll Da^{-1},$$

(1)

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where $D_n = d k_e u_n^{-1} c - T_n / T_0$ is the Damköhler number, $M = u_b / c$ is the Mach number, $d$ is the channel cross dimension, $k_e$ is the Arrhenius preexponential factor, and $T_n$, $T_b$ are the activation and burning temperatures, nondimensionalized by the initial temperature $T_0$ of unburnt gas mixture. The choice of the flame front speed relatively to the burnt gas $u_b = T_b u_n$ as the reference quantity for gas velocity components, makes Damköhler number dependent on other nondimensional complexes and implies the formula $D_n = \text{Re} Pr (T_b - 1)^2 T_n^2 / 2$, where $\text{Re} = \rho_0 u_b d / \mu$, and $Pr = \mu / \rho c_p \lambda$ are the Reynolds and Prandtl numbers correspondingly. In sequel, condition (1) can be rewritten as a limitation on the Reynolds number

\[ \text{Re} \ll \frac{2T_0^5}{M Pr (T_b - 1)^2 T_n^2}. \]  

(2)

From the physical point of view, this inequality means, that the relaxation time of acoustic processes should be much faster than that of the chemistry. Otherwise, generally speaking, first order terms of asymptotic expansions could grow, because of possible acoustic-kinetic interaction, up to the magnitude of the zero order terms, making the asymptotic expansions invalid.

The purpose of the present work is to develop efficient numerical algorithms to study flame evolution in closed channels for low, but distinct from zero, Mach numbers $M$ and for high Reynolds numbers $\text{Re}$, exceeding restriction (2). In order to fulfill this purpose, the system of Navier-Stokes equations for a compressible, chemically reacting gas mixture was chosen as the mathematical model. Numerical algorithms are based on upwind finite-difference schemes of high order approximation and employ locally preconditioned iterations in order to obtain solution to the implicit system of grid equations on each time step. An illustration of application of the approach is given in the final Section.

2 Mathematical model

The system of equations considered in this work describes dynamics of a gas mixture of species $A$ and $B$ in a closed channel induced by a model exothermic reaction $A \rightarrow B$ with Arrhenius reaction rate. It is based on the Navier-Stokes system for compressible gas accomplished by the balance equation of species $A$, and takes into account chemical heat release $q$ in the energy balance equation. Values of viscosity $\mu$, thermal conductivity $\lambda$, diffusivity $D$, specific heats ratio $\gamma = c_p / c_v$, and molecular weights are assumed to be constant and do not differ significantly from species to species. Gravity is set to zero. The system of governing equations can be written in the following conservative form

\[ \frac{\partial V}{\partial t} + \frac{\partial F^{(a)}}{\partial x_1} + \frac{\partial G^{(a)}}{\partial x_2} = \frac{\partial F^{(d)}}{\partial x_1} + \frac{\partial G^{(d)}}{\partial x_2} + H, \]  

(3)
where \( V = (\rho, \rho v_1, \rho v_2, \rho \mathcal{E}, \rho Y)^T \) are the conservative variables, \( \rho \) is the density, \( v_1, v_2 \) are the velocity components, \( \mathcal{E} = T / (\gamma - 1) + \gamma M^2 \left( v_1^2 + v_2^2 \right) / 2 \) is the total energy and \( Y \) is the fuel mass fraction. Adveotive fluxes \( F^{(a)} \), \( G^{(a)} \) and source term \( H \) are defined by the relationships

\[
F^{(a)} = \begin{pmatrix} \rho v_1 \\
\rho v_1^2 + \frac{\gamma T}{\gamma M^2} \\
\rho v_1 v_2 \\
\rho v_1 \left[ \frac{\gamma T}{\gamma - 1} + \frac{\gamma M^2}{2} \left( v_1^2 + v_2^2 \right) \right] \\
\rho v_1 Y \end{pmatrix},
\]

\[
G^{(a)} = \begin{pmatrix} \rho v_2 \\
\rho v_1 v_2 \\
\rho v_2 \left[ \frac{\gamma T}{\gamma - 1} + \frac{\gamma M^2}{2} \left( v_1^2 + v_2^2 \right) \right] \\
\rho v_2 Y \end{pmatrix},
\]

\[
H = \begin{pmatrix} 0 \\
0 \\
0 \\
\frac{\partial \mathcal{E}}{\gamma \partial \rho} \left( \frac{\rho Y e}{\gamma M^2} \right) \\
- \partial \rho Y \left( \frac{\rho Y e}{\gamma M^2} \right) \end{pmatrix},
\]

where the formula given in the Introduction should be used for the Damköhler number. Here the initial density \( \rho_0 \) and fuel mass fraction \( Y_0 \) of the unburnt mixture, the channel width \( d \) and value of \( d/u_0 \) were used as the reference quantities for the density, fuel mass fraction, length, and time correspondingly. Nondimensional value of reaction heat release is given by formula \( Q = qY_0/c_0 T_0 \). Expressions for dissipative fluxes \( F^{(d)} \), and \( G^{(d)} \) can be found somewhere else.

We consider system (3) in a rectangular domain \( \Omega = [0, L] \times [0, 1] \) for \( t \geq 0 \). Vanishing gas velocity and gradient of the fuel mass fraction normal to the walls are assumed as the boundary conditions. Walls are considered both thermo insulated and cooled to the given temperature \( T_w \). Combustion of the mixture is initiated by increasing the gas temperature in the initial conditions up to \( T_b \) in a few grid cells. Gas density and fuel mass fraction are considered in equilibria with the temperature distribution in the initial conditions, while initial gas velocities are set to zero for \( t = 0 \).

3 Numerical algorithms

Numerical solution of (3) by explicit finite-difference methods requires usually, that the time step \( \Delta t \) does not exceed some value \( \Delta t_{CFL} \sim M h \), where \( h \) is the size of the numerical grid cell. Difficulties arising from this limitation when the Mach number \( M \) tends to zero were recognised many years ago, see e.g. [Choi (93)]. It was found that implicit approximation of system (3) is not enough to weaken severe CFL time step restriction for low Mach numbers substantially. The failure of the implicit approximation in this case can be attributed to the poor initial guess provided by the solution on the current time level for the solution on the upper one. Thus, neither one Newton iteration,
used by implicit schemes, nor more of them give a satisfactory approximation for the solution on the upper time level. The situation can be illustrated by an example of a transcendental equation, e.g. \( \tanh \varepsilon z = x_0 \) for \( \varepsilon \ll 1 \), when Newton iterations converge for initial guesses \( x^{(0)} \in O(x_0) \) only. Employment of properly generalised Newton methods fixes the problem of the initial guess, but dramatically increases the number of iterations required to achieve a reasonable accuracy as \( M \to 0 \).

On the other hand, the system of finite-difference equations resulting from an implicit approximation of the initial boundary value problem for equations (3) can be effectively solved with a locally preconditioned iterative solver. In the case of fully implicit approximation, equations of the locally preconditioned iterative method take the form

\[
\begin{align*}
\frac{U^{(n+1,m)}_{i,j} - U^{(n+1,m-1)}_{i,j}}{\tau} + \frac{V^{(n+1,m)}_{i,j} - V^{(n)}_{i,j}}{\Delta t} \\
+ \frac{F^{(n+1,m)}_{i+1/2,j} - F^{(n+1,m)}_{i-1/2,j}}{\Delta x_1} + \frac{G^{(n+1,m)}_{i,j+1/2} - G^{(n+1,m)}_{i,j-1/2}}{\Delta x_2} = H^{(n+1,m)}_{i,j},
\end{align*}
\]

(4)

where \( m = 1, \ldots, m_0 \) is an iterative index, \( V^{(n+1,0)} = V^{(n)} \), \( V^{(n+1)} = V^{(n+1,m_0)} \), \( P \) is a preconditioner, \( \tau > 0 \) is an iterative parameter, \( F = F^{(a)} - F^{(d)} \), \( G = G^{(a)} - G^{(d)} \), and \( U = (\Delta p, v_1, v_2, T, Y)^T \). Also, \( n, i, \) and \( j \) are indexes of time \( t \) and space independent variables \( x_1 \) and \( x_2 \) correspondingly.

Note, that a new set of dependent variables \( U \) is used in (4) instead of \( V \). It uses splitting of pressure \( p = \rho T = P + \Delta p \) into “thermodynamic” \( P \) and “acoustic” \( \Delta p \) parts. Value of \( P \) is estimated for the \( (n+1) \)'s time level by using the overall balance of energy before the start of iterations (4). In the case of thermo insulated walls, the corresponding equation, see [Karlin (98)], is

\[
P = \frac{1}{L} \left( \int_0^L \int_0^1 p^{(n)} dx_1 dx_2 \right) e^{\frac{Q_{in}}{L} x_1} \int_0^1 \frac{v^{(n)}}{\sqrt{T^{(n)}}} e^{-\frac{Q_{in}}{L} x_1} dx_1 dx_2.
\]

During the iterations, the total pressure and density are kept updated in accordance to formulas \( \rho^{(n+1,m)} = p^{(n+1,m)}/T^{(n+1,m)} \) and \( p^{(n+1,m)} = P + \Delta p^{(n+1,m)} \). We emphasise, that equation (5) is not a part of the governing system, but is just an intermediate step in low round-off error evaluation of pressure gradient in (4).

Characteristic flux-difference splitting [Roe (81)] modified for the presence of local preconditioner \( P \) [van Leer (91)] and combined with upwind, high-order finite-difference approximations of inviscid fluxes [Chakravarthy (85)] were employed in this work. The overall formal order of approximation of this method is \( O(\tau^2 + h^2) \), if space derivatives in (4) are interpolated into the time level \( n + 1/2 \). In practice, equations (4) are linearised relatively to \( U^{(n+1,m)}_{i,j} - U^{(n+1,m-1)}_{i,j} \) and the finite-difference operator on the upper iterative level \( m \) is approximately factorized.
At present, many local preconditioners $P$ have been proposed and evaluated, see e.g. [Darmofal (96)]. We found that the preconditioner described in [Choi (93)] performs satisfactorily in the problems in question and used it in this work.

Really fast chemistry with $D_0 \gg M^{-1}$ may affect the convergence of iterations (4) so much, that splitting it into fractional step becomes useful, if not unavoidable. In doing so updating of $P$ by formula (5) and subsequent correction of $P = P + \Delta P$ for the initial guess of iterations (4) should be done after every chemical fractional step. In a particular case of a model $A \rightarrow B$ reaction, integration of the split kinetic system can be carried out analytically, resulting in an implicit transcendental equation involving the exponential integral. In general, corresponding initial value problems should be integrated numerically with a standard stiff ODE solver [Byrne (87)]. Symmetric splitting preserves the formal order of approximation at $O(r^2 + h^3)$.

4 Examples of computations and conclusion

Figure 1 shows flame front propagation in a closed channel for $M = 10^{-2}$, $Re = 200$, $Q = 7$, and $\tau_a = 33$ (in this case $D_0 = 350.12$). Five equidistant level lines are depicted, of mass fraction $Y$ in the range from 0.4 to 0.6 for a sequence of ten consecutive time moments starting from $t = 0$ with the interval 0.5. Solution was obtained by the method presented in this paper on a numerical grid of $513 \times 129$ nodes and with the time step $\Delta t = h/5$, where $h = 1/128$.

Solution of the same problem with the same discretization parameters, but within the low Mach number model, see [Makhviladze (94)], is presented in Figure 2, where the flame front is shown at the same instants as in Figure 1. The Figures reveal some slight, but visible differences in shape and velocity of propagation of the flame front calculated by two different methods. Further calculations show that these differences can be more pronounced for other values of governing parameters of the problem.

Generally speaking, by adapting implicit approximation of the problem with time steps drastically violating the formal CFL condition, we are no longer able to resolve acoustic perturbations properly, while there were not filtered out explicitly in contrast to the low Mach number model. Therefore, the question of which approach is more plausible remains open. Further conclusions can be made through comparative computations and experimental data analysis as well as through Navier-Stokes computations on high performance computers keeping to the CFL condition.

References

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Fig. 1. Navier-Stokes model with local preconditioner

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Fig. 2. Low Mach number model
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