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A new approach to simulate confined, premixed and slow combustion

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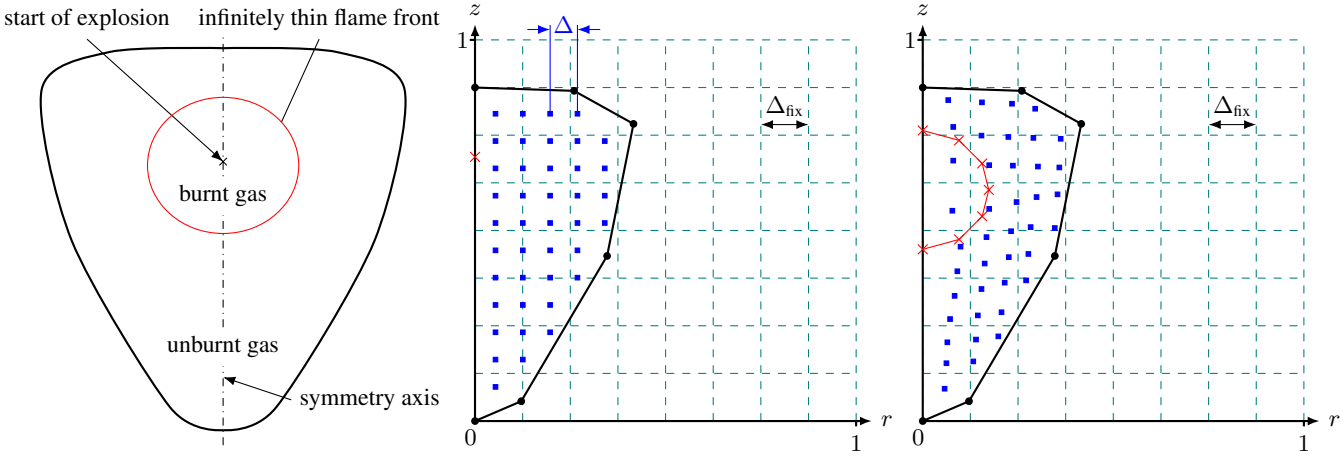
To simulate confined combustion, a new numerical method is presented. Assuming low-Mach number flow and neglecting viscosity, radiation and heat conduction, the divergence of the velocity field is time-dependent only. Thus, Helmholtz decomposition of the flow field yields a simpler numerical solution algorithm. This leads to Poisson's equations for the scalar and vector potential. To track the flame front, marker points are distributed along the discontinuity.

1 Physical Model

An ideal gas is inside a rotational symmetric vessel, see Fig. 1a. Radiation, heat conduction, heat loss to the surroundings and friction are neglected. After ignition, which can only occur along the symmetry axis, an infinitely thin flame front develops. The reaction enthalpy is part of the internal energy of the unburnt gas. The effective burning velocity, i.e. the velocity of a sufficiently smooth, averaged flame front w.r.t. the unburnt gas, depends on the local curvature $\tilde{\kappa}$ and thermodynamic state, $\tilde{s}_{\text{eff}} = (1 - \tilde{\kappa}\tilde{l}_{\text{t}}^{\text{stab.}})(\tilde{T}_{\text{u}}/\tilde{T}_{\text{ref}})^2(\tilde{p}_{\text{ref}}/\tilde{p})^{\beta}\tilde{s}_{\text{eff}}^0$. $\tilde{T}$ is the temperature, $\tilde{p}$ is the pressure, $\tilde{l}_{\text{t}}^{\text{stab.}}$ is a stabilisation length, β is the pressure-dependency coefficient and $\tilde{s}_{\text{eff}}^0$ is the effective burning velocity at reference state $(\tilde{T}_{\text{ref}}, \tilde{p}_{\text{ref}})$. More details on the physical model are given in [3, 4].



(a) A flame front inside a closed vessel. **(b)** Spatial discretisation at time $t = 0$. **(c)** Spatial discretisation at time $t > 0$.

Fig. 1: Illustration of a flame front inside a close vessel (left) and the spatial discretisation for two different times (middle, right) [4].

After inserting characteristic scaling quantities into Euler's equations[1], a non-dimensional parameter $\varepsilon = (\tilde{s}_{\text{eff}}^0)^2/(\tilde{p}_{\text{i}}/\tilde{\varrho}_{\text{i}}) = \text{M}_{\text{ref}}^2/\gamma$ appears. It is proportional to the square of a reference Mach number M_{ref}. Assuming low-Mach number flow, an asymptotic expansion for $\varepsilon \ll 1$ is sensible, e.g. $\varrho = \varrho_0 + \varepsilon\varrho_1 + \dots$. To get a closed problem, the leading-order governing equations and the second order momentum balance are needed:

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \vec{u}) = 0, \qquad \varepsilon \left(\frac{\partial \varrho \vec{u}}{\partial t} + \nabla \cdot (\varrho \vec{u}\vec{u}) \right) = -\nabla \left(P + \varepsilon p' \right), \qquad \frac{\partial \varrho e}{\partial t} + \nabla \cdot (\varrho \vec{u} e) = -\nabla \cdot (P\vec{u}) .$$

The index '0' has been dropped and P is the leading-order pressure, used in thermodynamic calculations, and p' is the second-order pressure. The second-order momentum balance is in red. Additionally, jump conditions are needed at the flame front (Eqs. (2.40) to (2.42) in [4]).

In leading order, the pressure is time-dependent only and the flow is isentropic, except at the flame front. Thus, the divergence of the flow field is also time-dependent only. Applying Helmholtz decomposition to the flow field $\vec{u} = \nabla\varphi + \nabla \times \vec{\psi}$

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[1] characteristic dimensionful scaling quantities: initial pressure $\tilde{p}_{\text{i}}$ and density $\tilde{\varrho}_{\text{i}}$, reference burning velocity $\tilde{s}_{\text{eff}}^0$, vessel diameter $\tilde{L}_{\text{ref}}$

yields Poisson's equations for the scalar φ and vector potential $\vec{\psi}$:

$$\nabla^2\varphi = \nabla\cdot\vec{u} = -\frac{1}{\varrho}\frac{\mathrm{D}\varrho}{\mathrm{D}t} = -\frac{1}{\gamma}\frac{1}{P}\frac{\mathrm{d}P}{\mathrm{d}t}, \qquad \nabla^2\vec{\psi} = -\nabla\times\vec{u} = -\vec{\omega}.$$

2 Numerical Implementation

Four different spatial discretisation schemes are used, as shown in Figs. 1b and 1c: (I) The flame front is tracked with marker points. (II) The vorticity transport equation is solved on a Lagrangian mesh. (III) The vector potential is found on a fixed Eulerian mesh using spectral methods. (IV) The vessel wall is discretised by panels, i.e. straight lines that form a polygon.

The scalar potential is split in three parts, $\varphi = \varphi_\mathrm{p} + \varphi_\mathrm{d} + \varphi_\mathrm{v}$. φ_p is a particulate solution, which is easily found. φ_d and φ_v fulfil the jump condition at the flame front and boundary condition at the vessel wall for the velocity, respectively. This is done by prescribing a singular volumetric line source along the flame front and vessel wall:

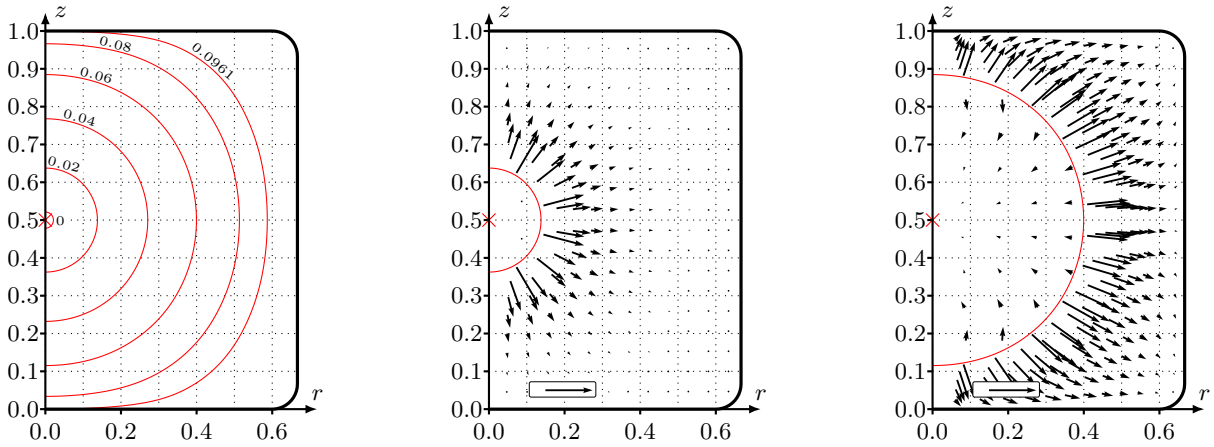
$$\vec{u}_\mathrm{p} = \nabla\varphi_\mathrm{p} = -\frac{1}{\gamma}\frac{1}{P}\frac{\mathrm{d}P}{\mathrm{d}t}\frac{\vec{x}}{3}, \quad \vec{u}_\mathrm{d} = \nabla\varphi_\mathrm{d} = \frac{\sigma-1}{4\pi}\oiint_\mathrm{FF}\frac{(\vec{x}-\vec{x}_\mathrm{f})\,s_\mathrm{eff}}{||\vec{x}-\vec{x}_\mathrm{f}||^{3/2}}\,\mathrm{d}O, \quad \vec{u}_\mathrm{v} = \nabla\varphi_\mathrm{v} = \frac{1}{4\pi}\oiint_\mathrm{KW}\frac{(\vec{x}-\vec{x}_\mathrm{v})\,q_\mathrm{v}}{||\vec{x}-\vec{x}_\mathrm{v}||^{3/2}}\,\mathrm{d}O.$$

q_v, the source strength distribution of the vessel wall, has to be determined such that the wall normal velocity vanishes. This resembles panel methods [1, 2] for internal flow.

The Poisson's equation governing the vector potential is found by expanding the vorticity and vector potential in a Fourier-Bessel series. Thus, the Laplace and curl operator are applied by performing algebraic operations on the Fourier-Bessel coefficients.

3 Results

Fig. 2 shows the position of the flame front for different times, and the flow field for two times. As soon as the flame touches the vessel wall, the simulation stops, at time $t = 0.0961$.



(a) Flame front positions. **(b)** Flow field for $t = 0.02$. **(c)** Flow field for $t = 0.06$.

Fig. 2: An explosion inside a cylinder with an aspect ratio of 0.75 and initial explosion at $z_\mathrm{i} = 0.5$ [4].

4 Discussion and Outlook

The presented numerical scheme makes use of the structure of the governing equations. The simulations account for flame-flow interaction and the influence of the vessel wall on the flame front. Major limitation of the model is that the stabilisation length scale $\tilde{l}_\mathrm{t}^\mathrm{stab.}$ remains unknown. The numerical treatment of the flame front requires a sufficiently large stabilisation mechanism, since the discontinuity has to remain smooth.

References

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