Microcombustor modeling using the RBF-FD method

M. Kindelan[1], V. Bayona[1], E. Fernández-Tarrazo[2] and M. Sánchez-Sanz[2]

[1]Mathematics Department
Universidad Carlos III de Madrid

[2]Fluid Mechanics Department
Universidad Carlos III de Madrid

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Micro rotary engine

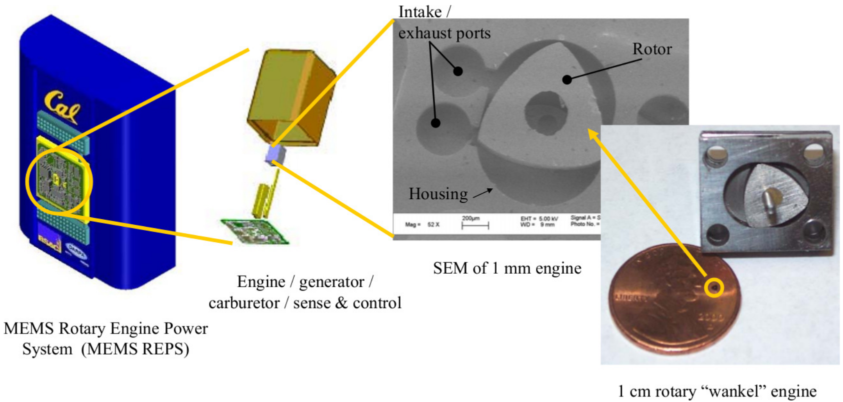


Figure : Sketch of a micro-rotary engine from the *Micro-Rotary Combustion Lab, University of California, Berkeley.*

Microscale combustion

- nano and micro technology devices require *compact* and *rechargeable* power supplies
- at present these devices rely on *batteries*
- but *energy density* of batteries is very low:
  - 0.7 MJ/kg for lithium-ion batteries
  - several hours to recharge
- possible alternative: *micro-engines*
  - hydrocarbon fuels have 45 MJ/Kg of stored chemical energy
  - an efficiency of 5% in converting this energy to electricity will outperform batteries
- small-scale *rotary engine* (Fernández-Pello, 2002)
  - high specific power
  - low cost due to: minimum number of moving parts and no valves required for operation
  - mechanical shaft output can be directly coupled to electric motor

Model

- Combustion chamber is approximated by a 2D channel.
- Bottom wall moves with velocity $\pm V$ relative to the other.
- Upper wall has a notch which modifies the combustible flow and facilitates the attachment of the flame.
- The velocity profile at the inlet is the sum of a Poiseuille flow and a Couette flow.
- When the mixture flows through the channel, a recirculation zone appears due to the notch.
- If the mixture is ignited, a steady flame might be established in the channel.
- Its structure and location depends on the flow rate which determines the attachment position, among other parameters.

Micro rotary engine: flow results

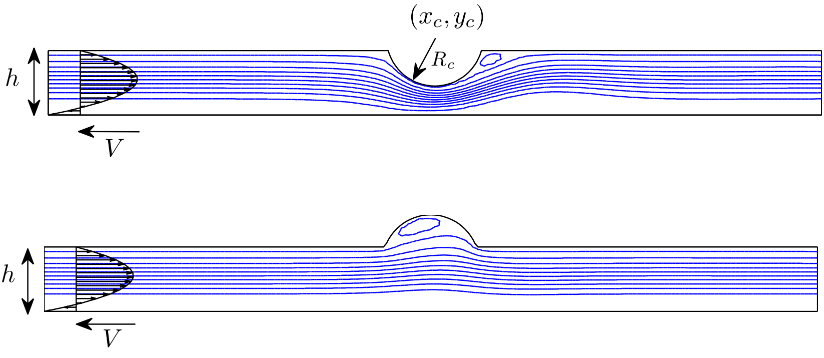
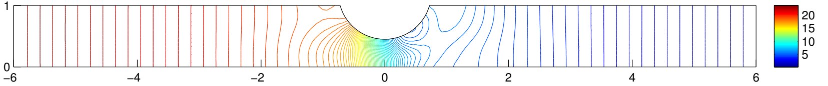


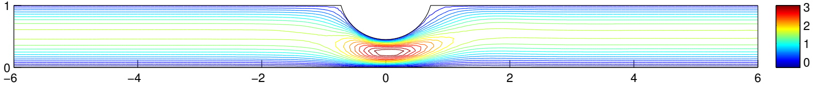
Figure : Channel configurations for an inner notch (up) and an outer notch (down). The flow field is illustrated by selected streamlines.

$m = 2$, wall velocity $V = -0.5$.

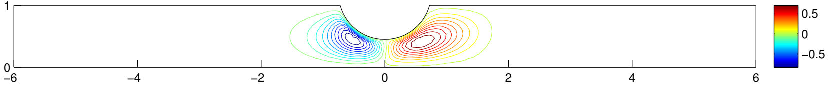
pressure



u velocity

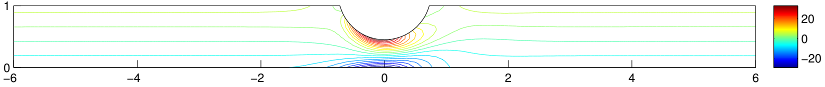


v velocity

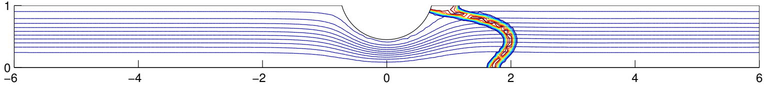


$m = 2$, wall velocity $V = -0.5$.

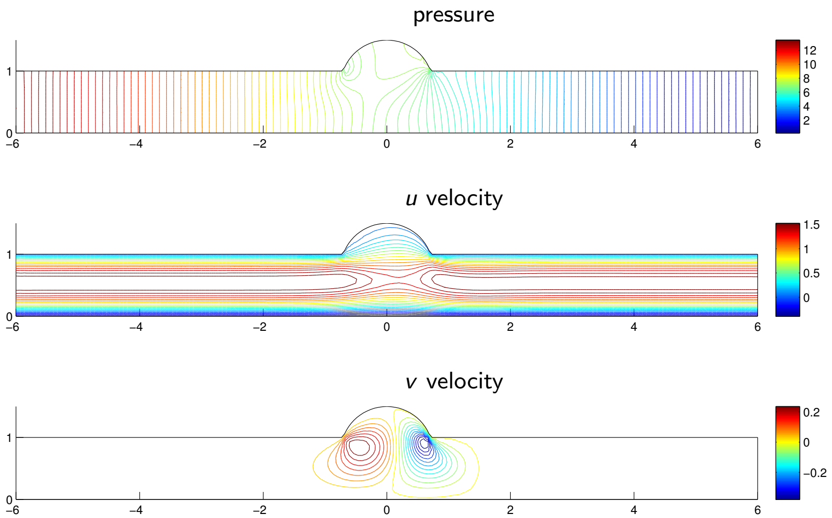
vorticity



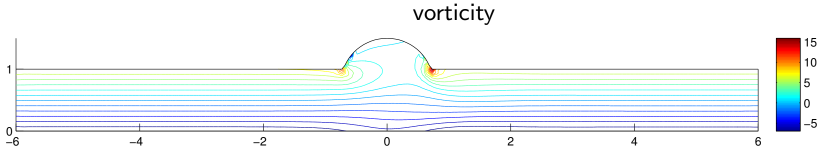
streamlines and reaction rate

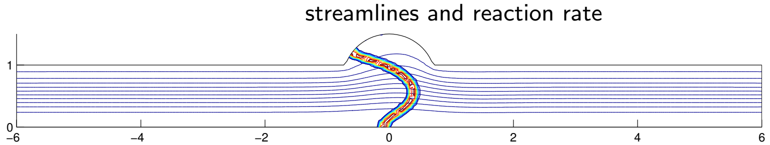


$m = 2$, wall velocity $V = -0.5$.



$m = 2$, wall velocity $V = -0.5$.





Parameters

m	mass flow
$Pr = 0.7$	Prandlt number
Pe	Peclet number
$Re = Pe/Pr$	Reynolds number
$Ze = 10$	Zeldovich number
$u_p = u_p(Le)$	S_L/U_L
$\gamma = 0.7$	heat release parameter
V	wall velocity
κ	heat loss coefficient
θ_m	temperature in combustion chamber

Thermo-diffusive model of flame propagation

The flow is assumed to be independent of the combustion, and is described by the continuity and momentum equations

$$\begin{cases} \nabla \cdot \mathbf{u} & = & 0 \\ (\mathbf{u} \cdot \nabla)\, \mathbf{u} & = & -\nabla p + \dfrac{1}{\mathrm{Pe}\,\mathrm{Pr}}\, \nabla^2 \mathbf{u} \end{cases} \tag{1}$$

The propagation of premixed flames subject to the previous flow is described by

$$\begin{cases} \dfrac{\partial \theta}{\partial t} + \mathrm{Pe}\, (\mathbf{u} \cdot \nabla)\, \theta & = & \nabla^2 \theta + \mathrm{Pe}^2\, \omega\, (\theta, Y) \\ \dfrac{\partial Y}{\partial t} + \mathrm{Pe}\, (\mathbf{u} \cdot \nabla)\, Y & = & \dfrac{1}{Le} \nabla^2 Y - \mathrm{Pe}^2\, \omega\, (\theta, Y) \end{cases} \tag{2}$$

where θ is the temperature, Y is the fuel mass fraction and $\omega(\theta, Y)$ is the reaction rate,

$$\omega\, (\theta, Y) = \frac{\mathrm{Ze}^2}{2\, Le\, u_p^2}\, Y \exp \left[\frac{Ze\, (\theta - 1)}{1 + \gamma\, (\theta - 1)} \right]. \tag{3}$$

Boundary conditions

$$y = 0: \qquad u = V, \;\; v = 0, \qquad \frac{\partial \theta}{\partial \vec{n}} = \kappa \, Pe \, (\theta - \theta_m), \quad \frac{\partial Y}{\partial \vec{n}} = 0,$$

$$y = y_s(x): \qquad u = v = 0, \qquad \frac{\partial \theta}{\partial \vec{n}} = 0, \qquad \frac{\partial Y}{\partial \vec{n}} = 0.$$

$$x \to -\infty, \qquad \begin{cases} u(y) = -6m\, y^2 + (6m - V)y + V, \quad v = 0 \\ Y = 1, \;\; \theta = \theta_m \end{cases}$$

$$x \to +\infty, \qquad \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0, \qquad \frac{\partial Y}{\partial x} = \frac{\partial \theta}{\partial x} = 0.$$

Domain and initial conditions

Channel length: $[L_0, L_f]$. Width $= 1$. Upper boundary:

$$y_s(x) = 1 + ae^{-bx^2}, \quad (4)$$

where a and b control the depth and width of the notch.
Initial conditions:

- Hot spot:

$$\begin{aligned} \theta(0) &= \theta_{ig}\, e^{-r^2/\delta^2}, \qquad r^2 = (x - x_{ig})^2 + (y - y_{ig})^2 \\ Y(0) &= 1 \end{aligned} \quad (5)$$

  where $x_{ig}, y_{ig}, \theta_{ig}$ and δ are parameters that define the location, intensity and decay rate of the initial hot spot

- Planar flame speed in channel (for $a = 0$):

$$\begin{aligned} Y(0) &= 1/\left(1 + e^{c(x+1)}\right) \\ \theta(0) &= \theta_m + (1 - \theta_m)(1 - Y(x)) \end{aligned} \quad (6)$$

Navier-Stokes equations

Stream function formulation,

$$u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x};$$

the Navier-Stokes equations take the form

$$\Delta^2 \psi + PePr \left[\frac{\partial \psi}{\partial x} \frac{\partial \Delta \psi}{\partial y} - \frac{\partial \psi}{\partial y} \frac{\partial \Delta \psi}{\partial x} \right] = 0 \tag{7}$$

with boundary conditions

$$y = 0 : \qquad \psi = 0, \qquad \frac{\partial \psi}{\partial \vec{n}} = V.$$

$$y = y_s(x) : \qquad \psi = m + V/2, \quad \frac{\partial \psi}{\partial \vec{n}} = 0.$$

As $x \to -\infty$,

$$\psi(y) = -2m\, y^3 + (3m - V/2)y^2 + Vy, \qquad \frac{\partial \psi}{\partial x} = 0. \tag{8}$$

As $x \to +\infty$,

$$\frac{\partial^2 \psi}{\partial x \partial y} = 0; \qquad \frac{\partial^2 \psi}{\partial x^2} = 0. \tag{9}$$

Navier-Stokes equations

Equation (7) is solved with Newton's method.

- Initial approximation $\psi^{(0)}$
- at each iteration compute $\psi^{(i)} = \psi^{(i-1)} + \xi$, where the correction ξ is the solution of

$$\Delta^2\xi + PePr\left[\frac{\partial\psi^{(i-1)}}{\partial x}\frac{\partial\Delta\xi}{\partial y} - \frac{\partial\psi^{(i-1)}}{\partial y}\frac{\partial\Delta\xi}{\partial x} + \frac{\partial\xi}{\partial x}\frac{\partial\Delta\psi^{(i-1)}}{\partial y} - \frac{\partial\xi}{\partial y}\frac{\partial\Delta\psi^{(i-1)}}{\partial x}\right] = R\left(\psi^{(i-1)}\right) \tag{10}$$

- with boundary conditions

$$B\xi = g(x,y) - B\psi^{(i-1)}. \tag{11}$$

- $R\left(\psi^{(i-1)}\right)$ is the residual at iteration i

$$R\left(\psi^{(i-1)}\right) = \Delta^2\psi^{(i-1)} + PePr\left[\frac{\partial\psi^{(i-1)}}{\partial x}\frac{\partial\Delta\psi^{(i-1)}}{\partial y} - \frac{\partial\psi^{(i-1)}}{\partial y}\frac{\partial\Delta\psi^{(i-1)}}{\partial x}\right], \tag{12}$$

- iterations continue until $\left\|R\left(\psi^{(i-1)}\right)\right\| \leq \epsilon$
- RBF-FD with polynomial augmentation is used to discretize differential operators.
- at each iteration equations (10) are solved using a direct solver.

Combustion equations

$$
\begin{aligned}
\frac{\partial \theta}{\partial t} &= \left[\nabla^2 - \mathrm{Pe}\,(\mathbf{u}\cdot\nabla)\right]\theta + \mathrm{Pe}^2\cdot\omega(\theta, Y) \\
\frac{\partial Y}{\partial t} &= \left[\frac{1}{Le}\nabla^2 - \mathrm{Pe}\,(\mathbf{u}\cdot\nabla)\right] Y - \mathrm{Pe}^2\cdot\omega(\theta, Y)
\end{aligned}
\tag{13}
$$

- Spatial differential operators: are discretized (in a preprocessing step) using RBF-FD augmented with polynomials. $\Rightarrow$ sparse differential matrices

$$
\begin{aligned}
D_\theta &= \nabla^2 - \mathrm{Pe}\,(\mathbf{u}\cdot\nabla)\,, \\
D_Y &= \frac{1}{Le}\nabla^2 - \mathrm{Pe}\,(\mathbf{u}\cdot\nabla)\,.
\end{aligned}
$$

Combustion equations

- Time integration: semi-implicit CN-AB2 (implicit for the linear terms and explicit for the non-linear terms).

$$\begin{aligned} \left(\mathbb{I} - \frac{\Delta t}{2} D_\theta\right) \theta^{k+1} &= \left(\mathbb{I} + \frac{\Delta t}{2} D_\theta\right) \theta^{k} + \frac{\Delta t}{2} \cdot \left(3G^k - G^{k-1}\right) \\ \left(\mathbb{I} - \frac{\Delta t}{2} D_Y\right) Y^{k+1} &= \left(\mathbb{I} + \frac{\Delta t}{2} D_Y\right) Y^{k} - \frac{\Delta t}{2} \cdot \left(3G^k - G^{k-1}\right) \end{aligned} \tag{14}$$

- (14) together with boundary conditions, are solved at each time step using iterative solver BiCGSTAB with iLU as preconditoner. G^k representes the non-linear term

$$G^k = \mathrm{Pe}^2 \cdot \omega(\theta^k, Y^k).$$

- Iterations continue until $\left\|\theta^k - \theta^{k-1}\right\| \leq \mathrm{tol}$ and $\left\|Y^k - Y^{k-1}\right\| \leq \mathrm{tol}$ ($\mathrm{tol} = 10^{-8}$).

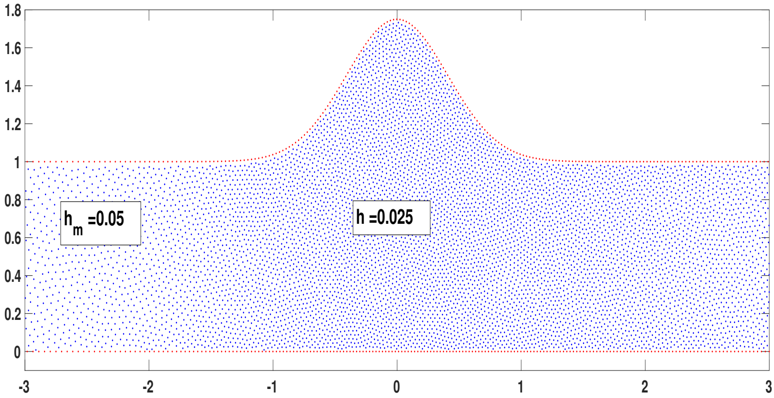
Domain discretization:

The domain is discretized using scattered nodes with an inter-nodal distance Δ controlled by a predefined function

$$\Delta = h + (h_m - h)\left[1/(1+\exp(2(x+3))) + 1/(1+\exp(-(x-3)))\right], \qquad (15)$$

where h_m and h are the inter-nodal distances away and near the notch, respectively. Ideally, a fine node distribution is used near the notch, becoming coarser towards the extremes of the channel.
A layer of ghost nodes is introduced all around the domain, so that:

1. the eight boundary conditions from the biharmonic equation (NS equations in the streamline formulation) can be satisfied.
2. The Runge phenomenon is avoided near boundaries.

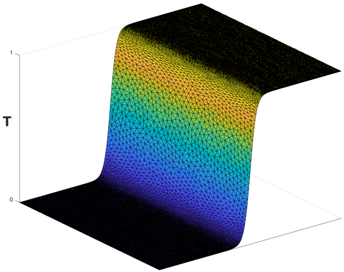


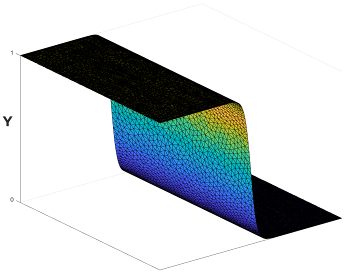
The spatial differential operators are approximated using PHS r^7 with polynomial augmentation up to m-th degree. The expected convergence is $O(h^m)$ for the combustion equations and $O(h^{m-2})$ for the biharmonic equation. V. Bayona, N. Flyer, B. Fornberg. G.A. Barnett, *J. Comput. Phys.* (2017).

Planar adiabatic flame

$$\begin{cases} \dfrac{\partial \theta}{\partial t} + u_p \dfrac{\partial \theta}{\partial x} = \Delta\theta + \omega \\ \dfrac{\partial Y}{\partial t} + u_p \dfrac{\partial Y}{\partial x} = \dfrac{1}{Le}\Delta Y - \omega \end{cases}$$

$$x \to -\infty, \quad \theta = Y - 1 = 0\,, \qquad x \to \infty, \quad \theta - 1 = Y = 0$$





Planar adiabatic flame, u_p vs Le

Fig 2 V. N. Kurdyumov, Combustion and Flame, 158 (2011)

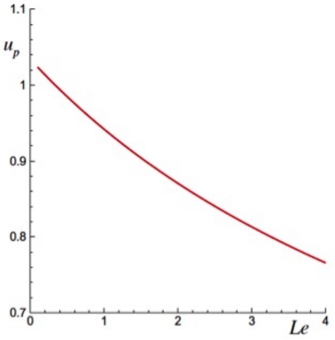


Fig. 2. Numerical values of factor $u_p = S_L/U_L$ appearing in Eq. (6) plotted as a function of the Lewis number for $\beta = 10$ and $\gamma = 0.7$. These values were kept in the present study.

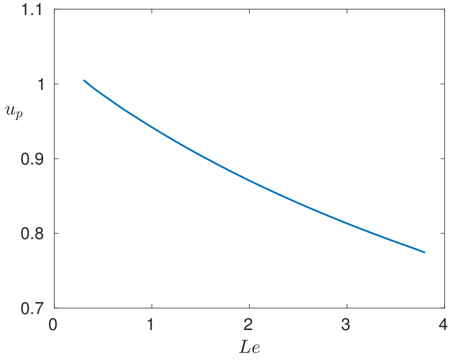


Figure : u_p vs Le

Premixed flame in flat channel

$$\begin{cases} \dfrac{\partial\theta}{\partial t} + \mathrm{Pe}\left[u_f(t) + 6m\,y\,(1-y)\right]\dfrac{\partial\theta}{\partial x} = \Delta\theta + \mathrm{Pe}^2\,\omega \\[2ex] \dfrac{\partial Y}{\partial t} + \mathrm{Pe}\left[u_f(t) + 6m\,y\,(1-y)\right]\dfrac{\partial Y}{\partial x} = \dfrac{1}{Le}\Delta Y - \mathrm{Pe}^2\,\omega \end{cases}$$

$$x \to -\infty, \quad \theta = Y - 1 = 0, \qquad x \to \infty, \quad \frac{\partial\theta}{\partial x} = \frac{\partial Y}{\partial x} = 0$$

$$y = 0, \quad \frac{\partial\theta}{\partial y} = \frac{\partial Y}{\partial y} = 0, \qquad y = 1, \quad \frac{\partial\theta}{\partial y} = \frac{\partial Y}{\partial y} = 0$$

Multiplicity of steady states: Le $= 0.7$, $m = 2$

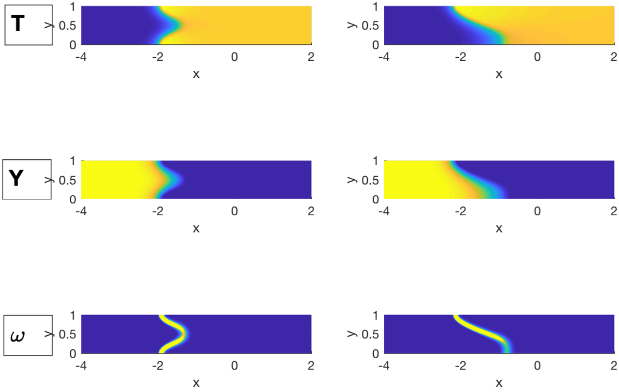


Figure : Symmetric (left) and non-symmetric (right) steady states.

Flat channel, u_f vs m

Fig 2 V. N. Kurdyumov, Combustion and Flame, 158 (2011)

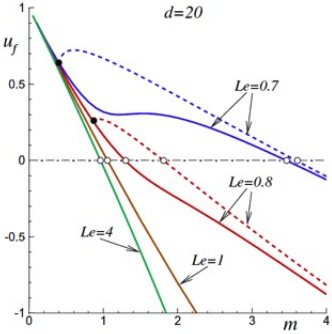


Fig. 3. Computed flame velocity $u_f = U_f/S_L$ as a function of the non-dimensional flow rate $m = U_0/S_L$ for several values of *Le* and $d = 20$; solid lines – symmetric flames; dashed lines – non-symmetric flames; the symbol • marks – the bifurcation points; the symbol ∘ – the critical flashback points.

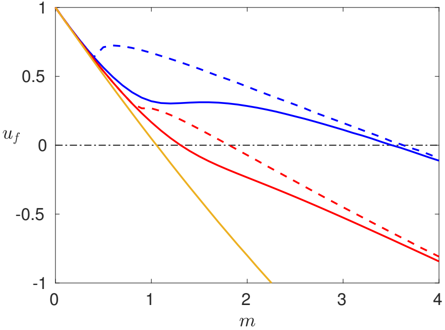


Figure : u_f vs m

Convergence

Convergence vs. h using polynomials of degree 2, 4, 6.

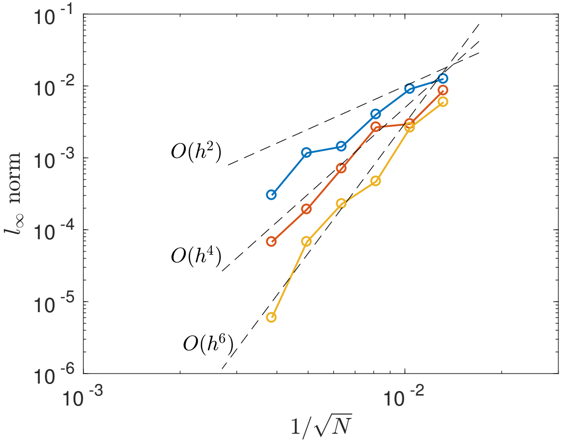


Figure : Convergence for $Le = 1$, compares against a solution obtained with $N = 310{,}209$.

Parameters

Table :

h_m	h	Δt	L_0	L_f	a	b	x_{ig}	y_{ig}	δ
0.05	0.025	$2\,10^{-6}$	-6	10	0.75	3	-1.25	0.2	0.15

V	m	Pe	Pr	Le	Ze	γ	κ	θ_m	θ_{ig}
2	2	10	0.7	1	7	0.7	-100	0	1

Isothermal, $V = 2$, $m = 2$, $x_{ig} = -1.25$, $y_{ig} = 0.2$

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Isothermal vs Adiabatic, $V = 2$, $m = 2$, $x_{ig} = -1.25$, $y_{ig} = 0.2$

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Isothermal, $V = 2$, $m = 2$, $y_{ig} = 0.2$

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$x_{ig} = -1.25$

$x_{ig} = -1.0$

Hot spot location for anchored flame

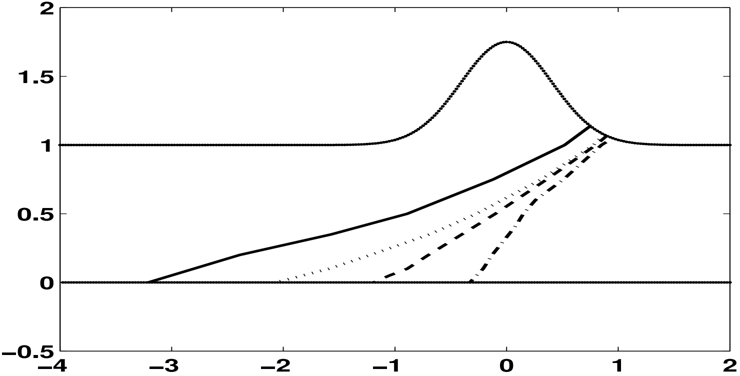

Figure : Each line separates locations of the hot spot for which the flame gets anchored (to the left) from locations in which it is blown up. Solid line: $m = 4$, $V = 0$. Dotted line: $m = 2$, $V = 2$. Dashed line: $m = 2$, $V = 0$. Dot-dashed line: $m = 2$, $V = -2$.

Conclusions

- Simplified model of time dependent combustion in microcombustor
- Model has been validated by computing flame velocity in a channel
- Polyharmonic splines with polynomial augmentation of m-th degree results in $O(h^m)$ convergence for steady solution
- Semi-implicit CN-AB2 for time integration
- Model yields information regarding
  - attachment of flame
  - location of hot spot for successful ignition
  - length of flame
  - fuel likeage
  - inner or outer notch, ...