Rich methanol combustion in small-scale counter-flow burners to produce hydrogen-rich syngas

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Introduction

In an effort to investigate the suitability of the concept of portable hydrogen production, rich methanol combustion (or partial oxidation) in a small-scale counter-flow burner consisting of an array of multiple narrow channels (see Fig. 1) is examined. The problem is described within the framework of a one-dimensional model (narrow-channel approximation [2]). Methanol oxidation is modeled with detailed chemistry and transport using the recently revised 247-step San Diego mechanism that involves $N = 50$ reactive species [1].

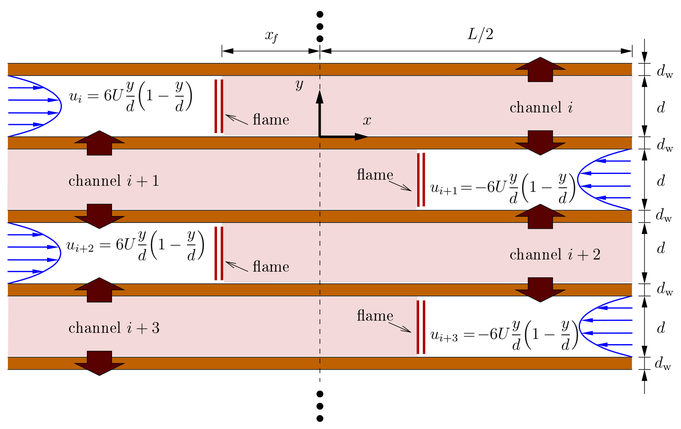

Fig. 1: Sketch of an array of multiple counter-flow narrow channels. L is the length of the channels, d is the distance between the internal surfaces of the walls, d_w is the thickness of the solid conducting walls, and x_f is half the distance between the opposed flames.

One-dimensional model

Assuming equal gas inflow velocity U_u in all channels (thus flames stabilize at symmetric positions $\pm x_f$ due to heat recirculation [3]), periodicity allows to reduce the analysis to a single channel i with the following governing gas-phase equations

$$\rho U = \rho_u U_u = \text{const.}, \tag{1}$$

$$\rho c_p U \frac{\mathrm{d}T}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\lambda_g \frac{\mathrm{d}T}{\mathrm{d}x}\right) - \rho \sum_{k=1}^{N} c_{p,k} Y_k V_k \frac{\mathrm{d}T}{\mathrm{d}x} - \sum_{k=1}^{N} \dot{\omega}_k h_k W_k - \frac{2\lambda_w}{d\, d_w}[T(x) - T(-x)], \tag{2}$$

$$\rho U \frac{\mathrm{d}Y_k}{\mathrm{d}x} = -\frac{\mathrm{d}}{\mathrm{d}x}(\rho Y_k V_k) + \dot{\omega}_k W_k, \qquad k = 1, 2, \ldots, N, \tag{3}$$

$$\rho = \frac{p\bar{W}}{\mathcal{R}T}, \tag{4}$$

and with the flux boundary conditions [4] at the left and right ends given by

$$x = -L/2 : \begin{cases} (\rho U h)_u = \rho U h - \lambda_g \dfrac{\mathrm{d}T}{\mathrm{d}x} + \displaystyle\sum_{k=1}^{N} \rho Y_k V_k h_k, \\ (\rho U Y_k)_u = \rho U Y_k + \rho Y_k V_k, \end{cases} \tag{5}$$

$$x = L/2 : \quad \frac{\mathrm{d}T}{\mathrm{d}x} = 0, \ \frac{\mathrm{d}Y_k}{\mathrm{d}x} = 0. \tag{6}$$

This one-dimensional formulation is identical to that describing the propagation of a planar flame, with U evaluated at the unburnt conditions being the flame propagation velocity. Here, however, $U(x) = \{\int_0^d u(x,y)\,\mathrm{d}y\}/d$ corresponds to the average flow velocity within the prescribed Poiseuille flow. The parameter $b = 2\lambda_w/(d\, d_w)$ appears in the energy equation as a volumetric heat-recirculation term and measures the amount of heat transfered across the dividing solid walls. For a micro-burner with $d = 4$ mm and $d_w = 1$ mm the order of magnitude of b lies typically within 10^5 W/(m^{3}K) for materials as quartz to 10^7 W/(m^{3}K) for silicon carbide [5].

Results

Two different lengths of the channels $L = 2$ cm and $L = 10$ cm are investigated. In Fig. 2 we depict the temperature and hydrogen molar fraction profiles along channel i for different equivalence ratios at a fixed inflow velocity. In Fig. 3 we plot them for different inflow velocities at a fixed equivalence ratio. We also plot in the figures (dot-dashed lines) the corresponding values for chemical equilibrium conditions for $\phi = 2, 3$ and 4.

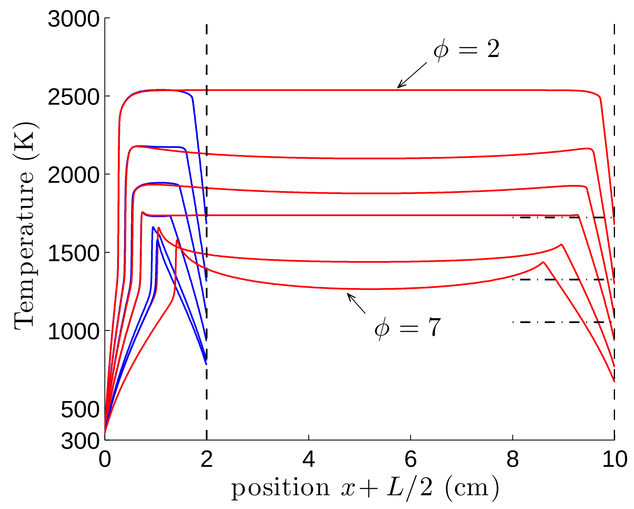

Fig. 2: Profiles of temperature and hydrogen molar fraction along channel i for $L = 2$ cm and $L = 10$ cm. Calculated for $\phi = \{2, 3, 4, 5, 6, 7\}$, $U_u = 200$ cm/s, $T_u = 343$ K, $p = 1$ atm, and $b = 10^6$ W/m^3 K.

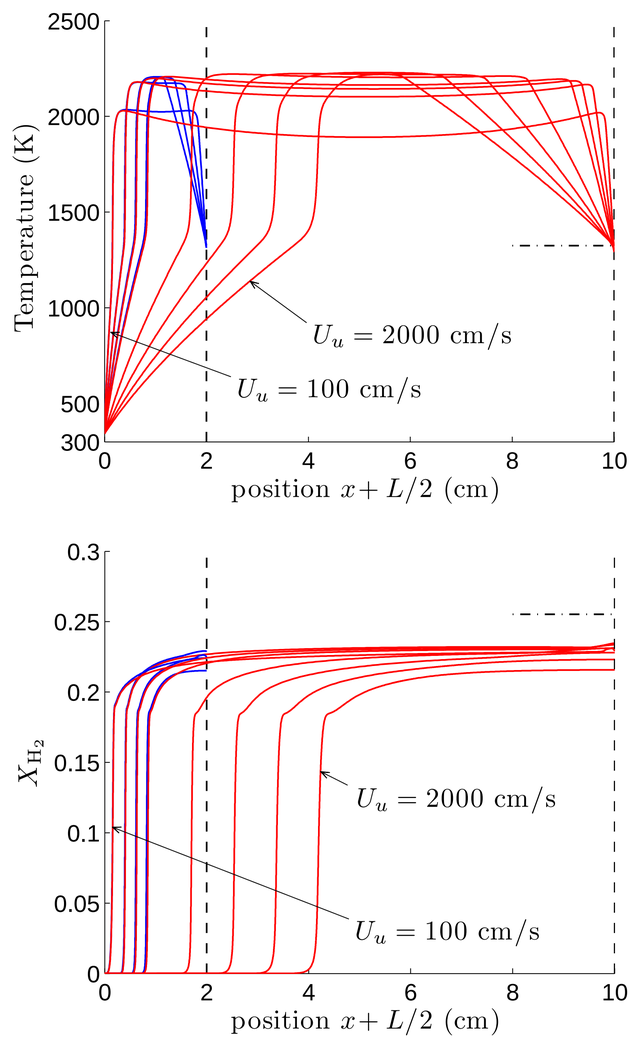

Fig. 3: Profiles of temperature and hydrogen molar fraction along channel i for $L = 2$ cm (dashed curves) and $L = 10$ cm (solid curves). Calculated for $U_u = \{100, 200, 300, 400, 800, 1200, 1600, 2000\}$ cm/s, $\phi = 3$, $T_u = 343$ K, $p = 1$ atm, and $b = 10^6$ W/m^3 K.

Figs. 4 and 5 show the conversion efficiency of methanol to hydrogen, defined, as in [5], as the ratio of H_2 moles produced per unit time at the exit of the reactor divided by the H_2 moles produced if all the atomic hydrogen bound in the fuel was converted to H_2. It is calculated as $\eta_{H_2} = \dot{N}_{H_2,\text{out}}/2\dot{N}_{CH_3OH,u}$, with $\dot{N}_j$ the molar flow rate of the species j. Maximum efficiency is found for equivalence ratios in the vicinity of 3 and inlet velocity of 200 cm/s.

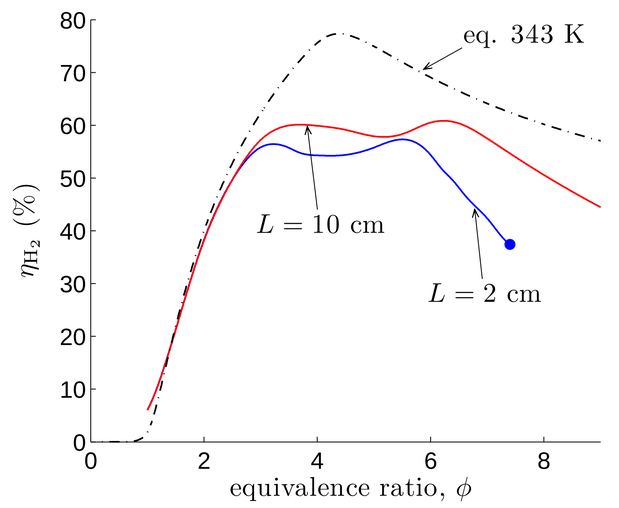

Fig. 4: Methanol-to-hydrogen conversion efficiency variation with the equivalence ratio. Calculated for $U_u = 200$ cm/s, $T_u = 343$ K, $p = 1$ atm, and $b = 10^6$ W/m^3 K. The dashed curve corresponds to equilibrium conditions. The solid circle indicates the blow-off limit (beginning of the unstable branch).

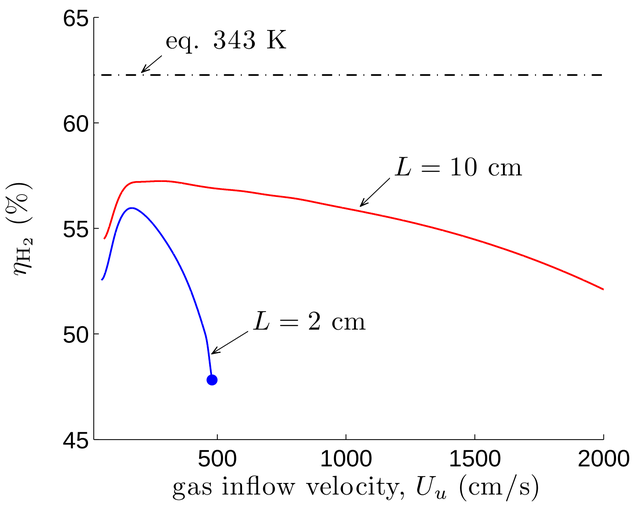

Fig. 5: Methanol-to-hydrogen conversion efficiency variation with the inlet velocity. Calculated for $\phi = 3$, $T_u = 343$ K, $p = 1$ atm, and $b = 10^6$ W/m^3 K.

Future work

- Study the effect of external heat losses.
- Study the effect of water addition (autothermal reforming)
- Investigate the effect of flame curvature (2D effects)

References

[1] "Chemical-Kinetic Mechanisms for Combustion Applications", San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego, Version 16-08-15, http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html.

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