

Numerical simulation of ethanol thermal partial oxidation in a mesochannel-based reactor to produce hydrogen-rich syngas

D. Fernández-Galisteo^{1*}, E. Fernández-Tarrazo², C. Jiménez¹, and V.N. Kurdyumov¹

¹Department of Energy, CIEMAT, Avenida Complutense 40, 28040, Madrid, Spain

²Departamento de Ingeniería Térmica y de Fluidos, Universidad Carlos III de Madrid, 28911, Leganés, Spain

(*) d.galisteo@ciemat.es

We examine numerically the ethanol thermal partial oxidation in an idealized configuration consisting of multiple counter-current channels separated by thin solid conducting walls. Within the framework of the narrow-channel approximation, the problem can be formulated as a one-dimensional model for a single channel with an extra term representing the heat transfer from the hot stream products to the fresh reactants in adjacent channels. Heat recirculation enables super adiabatic temperatures and promotes the oxidation of ethanol far beyond the conventional rich limit of flammability. The result is a feasible thermal partial oxidation process that produces hydrogen without the need for a catalyst. The idealized reactor shows hydrogen yields of 65% at equivalence ratios around 3.

Introduction

Fuel cell technology is increasingly considered as an alternative to conventional electrochemical batteries (e.g. lithium-ion batteries) to power small portable systems for long operating times [1]. Proton-exchange membrane fuel cells seem to be the most suitable due to the fast startup; however, they require pure hydrogen for operation. The production of hydrogen in situ from liquid fuels with high energy density is considered a promising alternative to the technically challenging hydrogen storage. In this work we investigate the suitability of the concept of portable hydrogen production in a mesochannel-based reformer that utilizes a biomass-derived fuel such as ethanol.

Among the main methods for hydrogen production from hydrogen-containing fuels, the simplest method to be applied in mesoscale channels is the partial oxidation method. To obtain large conversion rates of hydrogen in small-volume reactors, completion of the chemical process should be carried out within a short residence time. As the process is limited by the kinetics, catalytic coated layers are frequently employed to accelerate the reactions. In this work, we investigate the concept of heat recirculation as an alternative to catalyst.

Experimental works have demonstrated the feasibility of hydrogen production without catalyst using heat recirculation in a multiple mesoscale channel device with alternating flow directions. Ellzey et al. [2] used four parallel counter-current channels separated by silicon carbide walls to produce hydrogen-rich syngas from propane. Chen et al. [3] used a Swiss-roll burner.

Formulation of the problem

Consider ethanol-air partial oxidation in counter-current planar channels of width d and length L , as sketched in Fig. 1. The gas mixture is introduced at initial temperature $T_u = 343$ K to prevent condensation and velocity U_u . In the framework of the narrow-channel approximation (when $d \ll \delta_T$, being $\delta_T = D_T/S_L$ the thermal flame thickness, with D_T and S_L the thermal diffusivity and the burning velocity of the planar flame) the problem can be simplified to a one-dimensional form. Periodicity further simplifies the problem to the analysis of a single channel. The partial oxidation process in the gas phase is modeled with the 247-step San Diego mechanism.

With the above assumptions, the problem is reduced to the integration of the following governing equations:

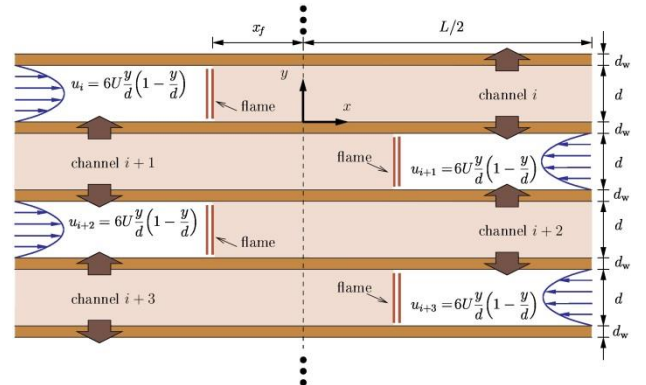


Figure 1. Sketch of the counter-current configuration.

$$\rho U = \rho_u U_u = \text{const.}, \quad (1)$$

$$\rho c_p U \frac{dT}{dx} = \frac{d}{dx} \left(\lambda_g \frac{dT}{dx} \right) - \rho \sum_{k=1}^N c_{p,k} Y_k V_k \frac{dT}{dx} - \sum_{k=1}^N \omega_k h_k W_k - \frac{2\lambda_w}{d} [T(x) - T(-x)], \quad (2)$$

$$\rho U \frac{dY_k}{dx} = -\frac{d}{dx} (\rho Y_k V_k) + \omega_k W_k, \quad k = 1, 2, \dots, N, \quad (3)$$

$$\rho = p_{atm} \bar{W} / (RT), \quad (4)$$

with the corresponding flux conditions at the left and right boundaries

$$x = -L/2: \begin{cases} \rho_u U_u h_u = \rho U h - \lambda_g \frac{dT}{dx} + \sum_{k=1}^N \rho Y_k V_k h_k, \\ \rho_u U_u Y_{k,u} = \rho U Y_k + \rho Y_k V_k, \quad k = 1, 2, \dots, N, \end{cases} \quad x = L/2: \quad \frac{dT}{dx} = 0, \frac{dY_k}{dx} = 0, \quad (5)$$

The parameter $b = 2\lambda_w/(d d_w)$ stands for the conductivity factor. In this work we consider a reactor of $L = 2$ cm long, $d = 4$ mm, $d_w = 1$ mm, and thermal conductivity of the silicon carbide, so that $b = 10^6$ W/(m³ K).

Results

Spatially resolved profiles of gas temperature, H₂ and CO mole fractions are presented in Fig. 2. We observe three different stages: 1) an inert preheating zone. 2) A reaction zone where the fuel is oxidized producing a large temperature increment and amount of H₂. We call primary the H₂ produced in this zone. 3) A post-oxidation zone where reforming occur, resulting in secondary H₂ formation. In Fig. 3 the efficiency of the reactor is depicted. In the point of maximum efficiency, a channel with a cross section of 16 mm² will produce a hydrogen mass flow rate of 0.7 mgr_{H₂}/s (85 W).

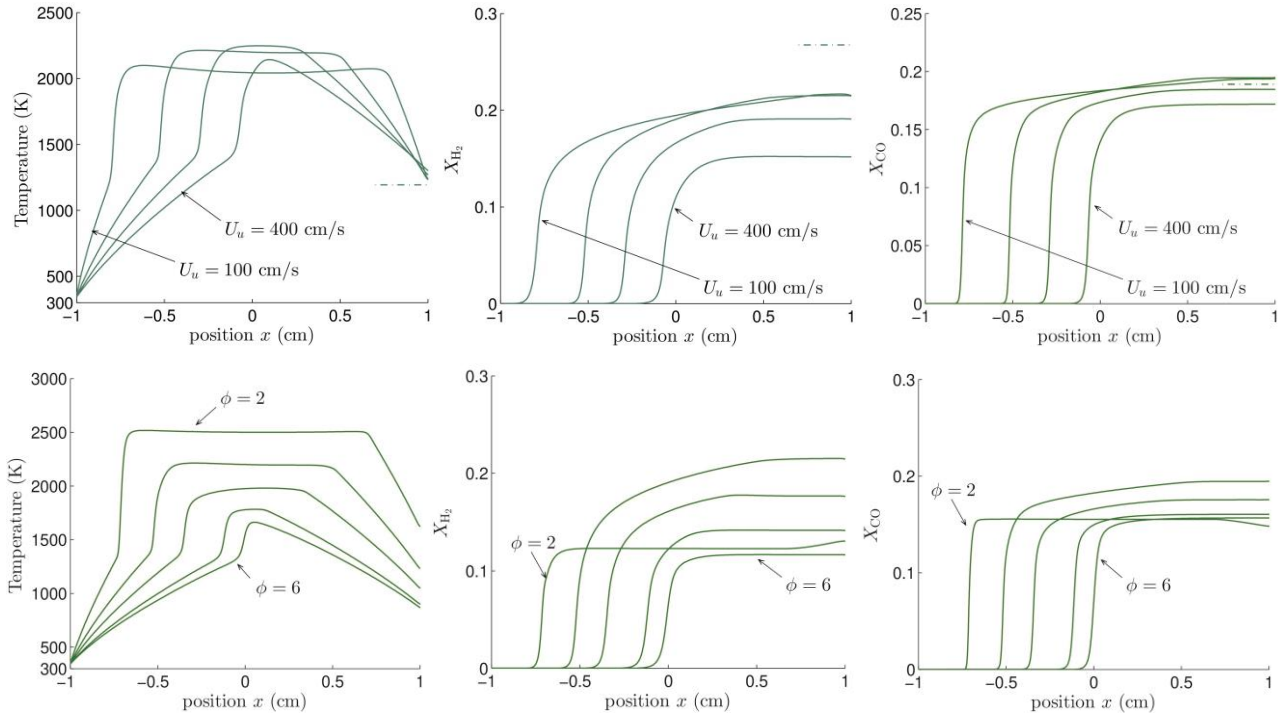


Figure 2. Profiles of gas temperature, H₂ and CO molar fractions calculated for inflow velocities $U_u = \{100, 200, 300, 400\}$ cm/s at fixed $\phi = 3$ (top); and for equivalence ratios $\phi = \{2, 3, 4, 5, 6\}$ at fixed $U_u = 200$ cm/s (bottom).

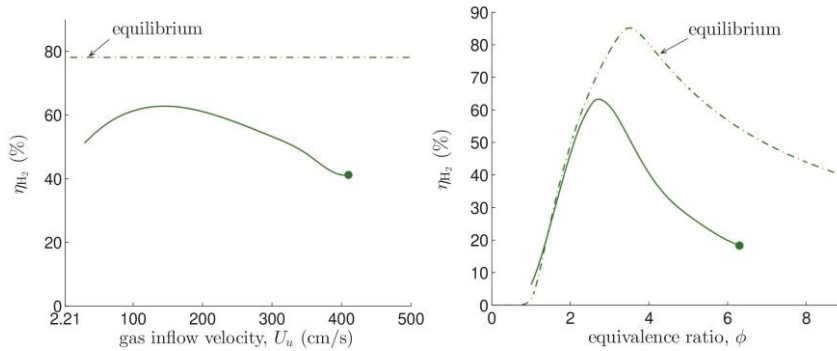


Figure 3. The H₂ yield at the exit of the reactor for fixed $\phi = 3$ (left) and for fixed $U_u = 200$ cm/s (right).

References

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