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Combustion stability and hetero-/homogeneous chemistry interactions for fuel-lean hydrogen/air mixtures in platinum-coated microchannels



Combustion and Flame

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ABSTRACT

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The hetero-/homogeneous combustion and stability limits of fuel-lean hydrogen/air mixtures (equivalence ratio $\varphi = 0.40$) were investigated numerically in a platinum-coated planar microchannel with a length of 10 mm and a height of 1 mm. A two-dimensional numerical model was used for both the gas and the solid, which included elementary heterogeneous and homogeneous reaction mechanisms, detailed transport, heat conduction in the solid, surface radiation heat transfer, and external losses via a heat transfer coefficient *h*. Pressures of 1 and 5 bar and solid thermal conductivities $k_s = 1$ and $16 \text{ Wm}^{-1}\text{K}^{-1}$ were analyzed, while stability maps were constructed in terms of the critical extinction heat transfer coefficient h_{cr} versus inlet velocity U_{IN} (or mass throughput). For a given solid thermal conductivity, there existed a crossover mass throughput above (below) which the stability envelope was broader at 5 bar (1 bar). Simulations with a surface perfectly stirred reactor (SPSR) model qualitatively reproduced the crossover points, which originated from a shift in the pressure dependence of the catalytic reactivity of hydrogen. For the low solid thermal conductivity $k_s = 1 \text{ Wm}^{-1}\text{K}^{-1}$, a non-monotonic dependence of the stability limits on the mass throughput was shown, with local minima created below the crossover point. The stability limits of hydrogen were solely determined by catalytic chemistry, as it sustained combustion at temperatures down to 320-380 K, at which gas-phase chemistry was frozen. Away from the critical extinction points, both catalytic and gas-phase reaction pathways were controlling. The diffusional imbalance of hydrogen, which led to catalytically-induced superadiabatic surface temperatures, and the suppression of the surface superadiabaticity by gaseous chemistry resulted in rich combustion phenomena, such as increasing peak wall temperatures with increasing heat transfer coefficients h. Critical extinction heat transfer coefficients for hydrogen were three to four orders of magnitude higher than those reported for methane and propane fuels in a similar channel geometry.

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1. Introduction

Hydrogen-rich fuels have attracted increased attention in combustion methodologies aiming at the reduction of CO_2 greenhouse emissions [1]. In particular, hydrogen combustion is of interest for post-combustion CO_2 capture approaches, wherein flue gas recycle (FGR) is typically applied to increase the CO_2 content in the exhaust gas and thus facilitate its subsequent capture [2]. With increasing amounts of FGR, however, combustion stability deteriorates. An option to restore combustion stability is the addition of hydrogen (produced e.g. via catalytic partial oxidation of part of the fuel [3]) into the diluted reactive mixture [4]. Another approach for reduced greenhouse emission is the pre-combustion CO_2 capture, which involves decarbonization of the fossil fuel

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(mainly coal, but also natural gas [5]) and subsequent combustion of a syngas mixture with high hydrogen content (> 80% vol.) [6,7]. Fundamental combustion characteristics of such syngas fuels are currently under intense investigation [8–10]. In addition to largescale power generation, hydrogen and hydrogen-rich fuels are also of interest for microreactors in portable power generation systems [11–14]. Such fuels can be produced from hydrocarbons using onboard microreformers [15–17].

For the aforementioned pre- and post-combustion CO_2 capture methodologies, hybrid concepts combining catalytic (heterogeneous) and gas-phase (homogeneous) combustion are under investigation. One such hybrid concept is the catalytically stabilized thermal combustion (CST) [18,19], in which part of the fuel is converted heterogeneously in a catalytic reactor and the rest is combusted in a downstream gas-phase burner. Both catalytic and gas-phase combustion modules in CST operate at fuel-lean stoichiometries. For pre-combustion CO_2 capture methods, the large amounts of hydrogen in the fuel mixture increase the risk of flame

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Nomenclature

- b channel half-height, Fig. 1
- specific heat at constant pressure of *k*-th gaseous $C_{p,k}$ species, Eq. (7)
- mixture-average diffusion coefficient D_{km} of *k*-th gaseous species, Eq. (6)
- D_{ν}^{T} thermal diffusion coefficient of k-th gaseous species, Eq. (6)
- view factor between discretized channel surfaces k F_{k-i} and *j*, Eq. (15)
- h total enthalpy, Eq. (4), heat transfer coefficient, Eqs. (12) and (18)
- h_k^0 chemical enthalpy of the k-th gaseous species, Eq. (7)
- Kg total number of gaseous species, Eq. (4)
- thermal conductivity of solid, Eqs. (8) and (9) ks
- total, catalytically-coated, and catalytically-inert L, L_a, L_i channel lengths, Fig. 1
- Lewis number (thermal over mass diffusivity) Le
- M_{S} total number of surface species, Eq. (11)
- р pressure, Eqs. (2) and (3)
- radiation heat flux on k-th discretized surface ele q_k ment, Eq. (14)
- radiation heat flux, Eq. (9) q_{rad}
- R universal gas constant, Eq. (7)
- catalytic molar production rate of k-th species, \dot{s}_k Eq. (9)
- S/Vsurface to volume ratio, Eqs. (17) and (18)
- Т temperature of gas
- T_r reactor temperature, Eq. (18)
- wall temperature, Eqs. (8), (9) and (12) TWALL
- reference temperature, Eq. (7) T_0
- ambient temperature, Eq. (18) T_{∞}
- streamwise velocity component Eqs. (1)-(3) и
- U_{IN} inlet streamwise velocity
- transverse (-y) velocity component, Eqs. (1)–(3)ν
- \vec{V}_k diffusion velocity vector of *k*-th gaseous species, Eq. (6)
- W_k, \bar{W} molecular weight of k-th gaseous species, average molecular weight
- mass fraction of k-th gaseous species Y_k
- streamwise and transverse coordinates, Fig. 1 х, у

Greek Symbols

k, *m*

WALL

wall

surface site density, Eq. (11) Γ δ_{s} thickness of solid wall, Fig. 1 surface emissivity, Eqs. (13) and (14) ε θ_m coverage of *m*-th surface species, Eq. (11) thermal conductivity of gas, Eq. (4) λ_g dynamic viscosity, Eqs. (2) and (3) μ ρ density of gas Stefan-Boltzmann constant, Eqs. (13) and (14) σ surface species site occupancy, Eq. (11) σ_m τ residence time, Eqs. (17) and (18) hydrogen-to-oxygen equivalence ratio φ homogeneous molar production rate of *k*-th species, $\dot{\omega}_k$ Eq. (5) Subscripts cr critical IN, OUT inlet, outlet

indices for gas-phase and surface species



Fig. 1. Catalytic channel geometry. All dimensions are in mm.

flashback. To this direction, the CST hybrid concept negates flashback due to the presence of the catalytic module, which in turn inhibits upstream flame propagation [20]. Conversely, for the postcombustion CO₂ capture methods, the catalytic reactor increases the combustion stability of the less-reactive FGR-diluted fuels by lowering their effective ignition activation energy [19]. While hybrid hetero-/homogeneous combustion is a possibility for largescale power generation, it is the preferred approach for microreactors. This is a result of the large surface-to-volume ratios of microreactors, the suppression of the various intrinsic flame instabilities in wall-bounded flows [21-25] by the presence of a catalyst [26,27], and the wider combustion stability envelopes of hetero-/homogeneous reactive systems compared to only homogeneous ones [28,29].

Recent studies have improved the understanding of gas-phase hydrogen kinetics, especially at elevated pressures relevant to power generation [8,30-32]. In addition, detailed mean-field catalytic reaction mechanisms for the oxidation of hydrogen on platinum (the catalyst of interest in the present study) have been developed [33-37]. Investigations of combined heterogeneous and homogeneous hydrogen combustion have also advanced. Appel et al. [38] employed in situ 1-D Raman measurements of major gas-phase species concentrations and 2-D laser induced fluorescence (LIF) of the OH radical in a Pt-coated channel and, in conjunction with numerical predictions, provided validated hetero-/homogeneous chemical reaction mechanisms for fuel-lean H₂/air mixtures at atmospheric pressure. Mantzaras et al. [39] and Ghermay et al. [40,41] extended the previous studies to pressures up to 15 bar, delineating the operating regimes where the competition between the two reaction pathways suppressed homogeneous combustion. Accompanying hetero-/homogeneous combustion experiments for fuel-rich H₂/air mixtures over Pt surfaces were reported in Schultze et al. [42]. In terms of simulations, fundamental hetero-/homogeneous kinetic studies were firstly reported by Bui et al. [43], who investigated the coupling of catalytic and gas-phase reactions for fuel-lean and fuel-rich H₂/air combustion in a stagnation point flow over a Pt surface at atmospheric pressure. Lately, Brambilla et al. [44] used 2-D direct numerical simulation (DNS) with conjugate heat transfer in the solid wall to study the transient combustion of fuel-lean H₂/air mixtures in a Pt-coated channel and to identify the main reactions controlling catalytic and gas-phase ignition.

Key issue in the design and thermal management of microreactors is the demarcation of stable combustion operating regimes. For gaseous combustion of methane/air and propane/air mixtures, stability was investigated numerically by Norton et al. [28,45] in channels with sub-millimeter gap sizes and chemically inert walls. They used 2-D simulations with a one-step gaseous reaction and assessed the impact of heat transfer mechanisms on the reactor energy management. For catalytic combustion of methane over Pt Download English Version:

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