



Direct numerical simulation of turbulent channel-flow catalytic combustion: Effects of Reynolds number and catalytic reactivity



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ABSTRACT

Three-dimensional direct numerical simulations of fuel-lean (equivalence ratio $\phi = 0.24$) hydrogen/air turbulent catalytic combustion were carried out in a platinum-coated planar channel with isothermal walls and an incoming fully-developed turbulent flow, at two inlet bulk Reynolds numbers ($Re_H = 5700$ and $12,360$ based on the channel height H) and four global catalytic reaction rates. The turbulent flow laminarization due to heat transfer from the hot catalytic walls was appreciable, with turbulent intensities dropping by 37% and 25% at the channel outlet for the low and high Re_H , respectively. The ratio of the local average turbulent hydrogen conversion rate to the corresponding local laminar conversion rate ($\langle \dot{s}_T \rangle / \dot{s}_L$) was found to be a monotonically increasing function of streamwise distance, Reynolds number Re_H , and catalytic reactivity. Despite the turbulent flow laminarization, $\langle \dot{s}_T \rangle / \dot{s}_L$ ratios at the channel outlet reached values up to 170% for the highest $Re_H = 12,360$ and for infinitely-fast catalytic chemistry. A correlation was further established for the ratio of the turbulent hydrogen conversion rate at finite-rate chemistry to the corresponding turbulent conversion rate at infinitely-fast chemistry. The instantaneous local catalytic reaction rates exhibited large fluctuations, which were up to 300% and 500% for the low and high Re_H , respectively. Fourier analysis indicated that a diminishing catalytic reactivity acted as a low-pass frequency filter for the overlying fluctuations of the turbulent flow.

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1. Introduction

Catalytic methods are cardinal for fuel processing technologies that convert the more abundant and low-cost natural gas to valuable fuels and chemicals [1]. This is accomplished either via the conventional indirect catalytic conversion processes (reforming of natural gas to syngas, followed by Fischer–Tropsch (F–T) synthesis of the desired chemicals [2]) or via the more recently investigated direct catalytic conversion processes such as oxidative coupling of methane (OCM) [3,4] or methane dehydroaromatization (MDA) [4]. Moreover, catalytic combustion is of interest for the latest power generation cycles targeting reduced greenhouse CO_2 emissions. In such cycles, post-combustion CO_2 capture can be efficiently accomplished through large flue gas recycle (FGR) in the reactant stream, which increases the CO_2 content in the exhaust gas and thus assists its subsequent capture [5]. The reduced reactivity of the FGR-diluted reactants calls for the use of catalytic combustion

methodologies due to their lower activation energy barrier that leads to enhanced combustion stability [6,7].

Catalytic reactors are typically made of ceramic or metallic honeycomb structures, comprising a multitude of channels (each with a hydraulic diameter of 1 to 2 mm) coated with an active catalyst. Turbulent flows inside the catalytic channels may occur especially at high operating pressures, which are relevant to both power generation and fuel processing applications. For example, at the high pressures of modern turbines (up to 30 bar) the inlet Reynolds numbers, based on the hydraulic diameter of an individual catalytic channel, can reach 20,000 [8]. For the commercially-relevant indirect route of natural gas conversion to chemicals, catalytic autothermal reforming is an option for syngas production. There are certain design advantages in carrying out the autothermal catalytic reforming and F–T synthesis at the elevated pressures dictated by the downstream F–T process. Furthermore, high pressure operation in the autothermal reformer significantly enhances the catalytic reactivity of methane towards (the upstream-occurring) total oxidation [9] while only modestly affecting the overall syngas yields and selectivities [10,11]. High-pressure operation, typically leads to high Reynolds numbers, requiring reliable numerical models

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for transitional or fully turbulent flows in catalytic channels. Such models are indispensable tools for reactor design and development in many industrial systems.

Modeling of turbulent flows in catalytic channels has been traditionally based on simple 1-D closures with lumped transport parameters (turbulent Nusselt and Sherwood numbers) [12]. Three-dimensional large eddy simulation (LES) has also been applied to a single monolithic catalytic channel of an automotive converter to investigate the transport-limited conversion (i.e. infinitely-fast catalytic chemistry) of the CO pollutant [13]. Detailed heterogeneous (catalytic) and homogeneous (gas-phase) chemistries have been implemented in turbulent channel-flow catalytic combustion modeling, adopting Low-Reynolds number (LR) submodels within the Reynolds Averaged Navier Stokes (RANS) description, along with appropriate surface/gas-phase chemistry closures [14,15]. Comparisons of model predictions with 1-D Raman measurements of major gaseous species concentrations across a catalytic channel boundary layer and with planar Laser Induced Fluorescence (LIF) of the OH radical have shown [14] that the combustion processes crucially depend on the turbulent flow laminarization induced by the heat transfer from the hot catalytic walls.

Three-dimensional Direct Numerical Simulation (DNS) of lean H_2 /air combustion in a platinum-coated catalytic channel with an inlet bulk Reynolds number (based on the channel height) of 5700 (friction Reynolds number $Re_\tau = 182$) was reported in Lucci et al. [16], using a global catalytic reaction and a prescribed wall temperature of 960K, which was sufficiently low to guarantee the absence of gaseous combustion. The foregoing study demonstrated the effect of flow laminarization on catalytic combustion, established that the fluctuations of the surface reaction rates had temporal frequencies comparable to the thermal response frequencies of typical solid materials used in catalytic reactors, and finally assessed limitations of RANS submodels. More recently [17] we reported DNS with detailed hetero-/homogeneous chemistry in the same channel and same inlet friction Reynolds number as in [16] at elevated wall temperatures of 1250–1270K in order to study the onset of homogeneous ignition and the conditions leading to local flame extinction.

In our earlier study [16] the chemical rate (global catalytic step) and the turbulence (Reynolds number) were fixed, thus limiting detailed investigations of the turbulence/chemistry interactions. The present work employs 3-D direct numerical simulations to study the turbulent catalytic combustion of fuel-lean H_2 /air mixtures in a plane channel at two inlet bulk Reynolds numbers ($Re_H = 5700$ and 12,360) and four global catalytic rates, with one of them corresponding to the transport-limited solution (infinitely-fast surface chemistry) and another to the chemically-inert case (no surface reactions). The main goal is to assess the impact of varying turbulence levels and chemical time scales on the resulting fluctuations of the surface reaction rates. By reducing the rate of surface chemistry at a given Reynolds number, the suppression of the temporally-fast catalytic rate fluctuations (which are in turn dictated by the overlying temporally-fast fluctuations of the normal-to-wall turbulent scalar transport) can be assessed. Alternatively, by increasing the Reynolds number at a given chemical reaction rate, the extent of departure from complete conversion of the limiting reactant (i.e. finite-rate chemistry effects) at the catalytic surface and the suppression of flow laminarization can be evaluated. Finally, the increase of the average catalytic rates due to turbulence can be assessed by comparing the DNS predictions with corresponding laminar-flow simulations.

This article is organized as follows. The governing equations, kinetic model, operating conditions and simulation domain are introduced in Section 2. Main results are presented in Section 3, starting with the turbulent flow laminarization in Section 3.1 and the underlying turbulence–chemistry interactions in Section 3.2.

Average turbulent catalytic rates are calculated and compared to corresponding laminar rates in Section 3.3, while turbulent catalytic rate fluctuations are elaborated in Section 3.4. Finally, conclusions are summarized in Section 4.

2. Numerical approach

2.1. Governing equations

The gas-phase is described by the low-Mach-number conservation equations for mass, momentum, energy and species in an open system ignoring gravity [18,19].

Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{u}) = 0 \quad (1)$$

Momentum

$$\rho \left(\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \nabla \underline{u} \right) = -\nabla p_1 + \nabla \cdot (\mu \underline{S}) \quad (2)$$

$$\underline{S} = \nabla \underline{u} + (\nabla \underline{u})^T - \frac{2}{3} (\nabla \cdot \underline{u}) \underline{I} \quad (3)$$

Energy

$$\rho c_p \left(\frac{\partial T}{\partial t} + \underline{u} \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) - \rho \left(\sum_{i=1}^{N_g} c_{p,i} Y_i \underline{V}_i \right) \cdot \nabla T \quad (4)$$

$$c_p = \sum_{i=1}^{N_g} Y_i c_{p,i} \quad (5)$$

Gas-phase species

$$\rho \left(\frac{\partial Y_i}{\partial t} + \underline{u} \cdot \nabla Y_i \right) = -\nabla \cdot (\rho Y_i \underline{V}_i), \quad i = 1, \dots, N_g \quad (6)$$

with N_g the total number of gaseous species.

Surface species

$$\frac{\partial \theta_k}{\partial t} = \sigma_k \frac{\dot{S}_k}{\Gamma}, \quad k = 1, \dots, N_s \quad (7)$$

with θ_k the coverage, σ_k the site occupancy and \dot{S}_k the catalytic molar production rate of the k th surface species, Γ the surface site density and N_s the total number of surface species.

Equation of state

$$p_0 = \frac{\rho RT}{\bar{W}} \quad (8)$$

where

$$\bar{W} = \left(\sum_{i=1}^{N_g} \frac{Y_i}{\bar{W}_i} \right)^{-1} \quad (9)$$

is the mean molecular weight of the gas mixture, and R the universal gas constant.

In order to filter out the acoustic waves and allow for longer integration time steps, the pressure in the low Mach number formulation is decomposed to a leading order term p_0 (thermodynamic pressure) and a first order term p_1 (hydrodynamic pressure appearing in the momentum Eq. (2)).

In the low-Mach-number formulation, Eq. (1) is replaced by Eq. (10) below, which is obtained by combining the continuity (Eq. (1)), energy (Eq. (4)), species (Eq. (6)) and state (Eq. (8)) equations:

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