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Extinction characteristics of catalyst-assisted combustion in a stagnation-point flow reactor

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Abstract

As a fundamental study to understand physical and chemical characteristics in catalyst-assisted combustion, numerical simulations of a stagnation-point flow combustor with a catalytic surface are performed. The combustible mixture of methane and air is blown on top of a platinum surface, forming a classical stagnation-point flow configuration. This geometry not only represents an on-chip microcombustor considered in recent studies, but it also serves as a canonical problem of combined heterogeneous/homogeneous combustion subjected to flow straining, which is a key parameter that governs the quenching and flammability limit. One-dimensional similarity formulation is derived with full consideration of detailed surface and gas-phase chemical kinetic models. Parametric studies are conducted to investigate the effects of strain rate, equivalence ratio, heat loss on the combustion, and extinction modes. The steady results showed that catalysis can largely extend the extinction limit, while suppressing the gas-phase reaction at lower strain rates. It was also found that the extension of the catalytic reaction quenching limit is sensitive to the mixture composition, suggesting the dominance of chemical aspects in catalytic combustion. The temperature versus strain rate response curves exhibit multiple branches of stable solutions, implying a possibility of hysteresis behavior in a coupled homogeneous–heterogeneous reactor. Extensive parametric studies in terms of the mixture equivalence ratio and the conductive heat loss parameter have revealed three distinct steady response regimes: a surface-dominant monotonic response, continuous two-branch response, and separated response showing an isolated surface-reaction island. The results are expected to provide insight into improving the overall combustion stability and efficiency of catalyst-assisted combustors.

Keywords: Catalytic reaction; Stagnation-point flow; Extinction; Microcombustion

1. Introduction

With the recent advances in the fabrication technologies for micro-electro-mechanical systems (MEMS), there is strong research interest in developing miniature power generation systems with a dimension ranging from a few centimeters to a fraction of a millimeter. Among many alternative energy sources for this application, combustion appears to be the most effective means in favor of its high-energy density, portability, and low adverse environmental impact [1].

In the design of a practical microcombustor, one of the major challenges in combustion aspects is to achieve a stable chemical reaction in a device that suffers from a large amount of heat loss due to its high

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Nomenclature

α	Damping coefficient
δ	Thickness of substrate
$\dot{q}$	Heat flow on the surface
$\dot{s}_k$	Molar generation rate of kth surface species
Γ_n	Surface site density for site type n
λ	Heat conductivity of gas
μ	Dynamic viscosity
ν	Ratio of surface to gas-phase activation temperatures
ω_k	Molar generation rate of gas-phase species k
ϕ	Equivalence ratio
ρ	Density
τ_g	Characteristic time scale of gas-phase reaction
τ_s	Characteristic time scale of surface reaction
c_p	Specific heat at constant pressure
E	Activation energy
h_k	Enthalpy of formation of species k
k	Conductivity heat transfer coefficient
K_g	Number of gas-phase species
K_s	Number of surface species
L	Length of computational domain
p	Pressure
p_∞	Inlet pressure
r	Radial coordinate
R^0	Universal gas constant
S	Strain rate
T	Temperature
T_∞	Inlet temperature
T_a	Activation temperature
u	Axial velocity
u_r	Reference axial velocity
U_∞	Inlet velocity
u_st	Stefan velocity
V	Radial velocity normalized by radial coordinate
v	Radial velocity
V_k	Diffusion velocity of species k
W_k	Molecular weight of species k
X	Mole fraction
Y_k	Mass fraction of species k
$Y_{k\infty}$	Inlet species mass fraction

surface-to-volume ratio. It is well known that combustion cannot be sustained in a dimension smaller than the quenching distance due to the overwhelming heat loss compared to the heat generated by the flames. To overcome this difficulty, catalytic materials are used as a means to sustain and stabilize combustion in the presence of large surface area [2–9]. In fact, catalytic technology has long been used in automotive applications to process postcombustion gases to reduce emissions. Catalytic combustion has also been used in gas turbines to achieve low-temperature stable combustion to reduce NOx [10,11]. In the microcombustor application, catalytic materials embedded on the reactor surface can extend the quenching limits so that stable combustion can be achieved under conditions that are otherwise nonflammable. Therefore, unlike the large-scale catalytic combustor, development of microcombustors faces drastically different challenges in identifying optimal operating conditions and meeting design targets. For example, achieving self-sustained combustion to overcome the quenching distance may be more important than establishing low-temperature and low-NOx combustion as would be the case in gas turbine applications. In a premixed combustion mode, increased viscous friction due to reduced dimension has also been found to be an additional source of combustion instability [12]. Therefore, it is of great interest to understand the fundamental characteristics of the coupled effects of surface and gas-phase chemical reactions that are more relevant in the microcombustor application.

In the present study, a stagnation-point flow is used as a model problem. This configuration has not only been considered as an on-chip microcombustor design [13] but it also serves as an excellent canonical configuration in which the coupling of surface and gas-phase combustion can be extensively investigated over a wide range of physical parameters, such as the equivalence ratio, flow strain rates, and heat loss to the surface. Extensive numerical calculations of steady flame behavior are performed using detailed reaction mechanisms [14] that have been validated against experimental measurements.

A number of asymptotic analyses have been performed for a stagnation-point flow configuration employing simple chemistry. An earlier study by Law and Sivashinsky [15] showed that the catalytic extension of the extincting limit of a stretched premixed flame is possible when the Lewis number of the deficient reactant is less than unity. Margolis and Gardner [16] analyzed a similar system in the near-unity Lewis number limit, considering both surface reaction and volumetric heat loss, and showed that catalytic reaction can significantly extend the extinction limits caused by flame stretch and heat loss. In addition, they found that multiple solution branches appear, corre-