

UC Davis

Mechanical and Aerospace Engineering

Title

Catalytically stabilized combustion of propane in heat-recirculating continuous flow reactors for improved flame stabilization and energy efficiency

Permalink

<https://escholarship.org/uc/item/7r8121jh>

Authors

Brown, Christopher
Chen, Junjie

Publication Date

2023-11-01

Supplemental Material

<https://escholarship.org/uc/item/7r8121jh#supplemental>

Data Availability

The data associated with this publication are available upon request.

Catalytically stabilized combustion of propane in heat-recirculating continuous flow reactors for improved flame stabilization and energy efficiency

Christopher Brown^a, Junjie Chen^{a, b, c, *}

^a Department of Mechanical and Aerospace Engineering, College of Engineering, University of California, Davis, California, 95616, United States

^b Department of Automotive Engineering, School of Mechanical and Automotive Engineering, South China University of Technology, Guangzhou, Guangdong, 510641, P.R. China

^c Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, 454000, P.R. China

* Corresponding author. E-mail address: junjiem@tom.com

Abstract

Flame stabilization is a common problem in small-scale combustion systems. However, the fuel-air mixture flow pattern, including any recirculation, is critical to achieving flame stability. In the present study, numerical simulations are conducted to understand the mechanisms of flame stabilization in heat-recirculating continuous flow reactors. The essential factors affecting combustion characteristics and flame stability are determined in order to obtain design insights. The results indicate that the wall thermal conductivity, flow velocity, equivalence ratio, and exterior heat losses are important factors in determining the energy efficiency of the reactor. There is an optimum wall thermal conductivity in terms of flame stability. The system with a moderate wall thermal conductivity will be most robust against the surrounding conditions. Excess enthalpy combustion can occur in an efficient and rapid manner, resulting from the injection of free radicals and heat produced by the catalytic reaction. The design incorporates the best features of both catalytic combustion and thermal flame methods. The system is essentially free of mass transfer limitations. Stable operation of the system is limited to a relatively wide flow regime, and the flow velocity is critical to achieving flame stability. Blowout shifts homogeneous combustion downstream significantly without substantially reducing the reaction rate. Both chemical and thermal environments are improved with the catalytically stabilized combustion method and the heat-recirculating structure.

Keywords: Flame stabilization; Catalytically stabilized combustion; Combustion characteristics; Energy efficiencies; Thermal flames; Excess enthalpy combustion

1. Introduction

A number of combustion systems promote partial conversion of a fuel followed by complete combustion of that fuel in a downstream combustion zone [1, 2]. These methods generally comprise introducing a fuel and air mixture into a combustion zone wherein a portion of the fuel has been partially reacted prior to entering the combustion zone. Such partial reaction may be promoted chemically, catalytically, or by any other conventional means depending upon each particular application [1, 2]. As the partially reacted fuel and air mixture are introduced into a region of the combustion zone, as with a dump, a flame is established to promote complete combustion of the fuel within the fuel and air mixture.

Flame stabilization is a common problem in these combustion systems [3, 4]. A flame will propagate through a fuel-air mixture only when certain conditions prevail. Initially, a minimum percentage of fuel must be present within the fuel-air mixture to make the fuel-air mixture flammable; the lean flammability limit [5, 6]. Similarly, a maximum percentage of fuel must be present within the fuel-air mixture wherein greater than this percentage will prevent burning; the rich flammability limit [5, 6]. The flammability range of a fuel-air mixture is that range of the percentage of fuel within the fuel-air mixture between the lean flammability limit and the rich flammability limit.

The stoichiometry of a fuel-air mixture contributes to its flammability range. A stoichiometric fuel-air mixture composition contains sufficient oxygen for complete combustion thereby releasing all the latent heat of combustion of the fuel. The strength of a fuel-air mixture composition typically is expressed in terms of its equivalence ratio; the equivalence ratio being the actual fuel-air ratio divided by stoichiometric fuel-air ratio. For example, an equivalence ratio of one represents a stoichiometric fuel-air mixture composition. An equivalence ratio less than one represents a lean mixture and an equivalence ratio greater than one represents a rich mixture.

Pressure and temperature contribute to the flammability range of fuel-air mixtures [7, 8]. Typically, with increases in pressure, the rich flammability limit is extended thereby extending the flammability range of the fuel-air mixture. Temperature, on the other hand, partially defines the flammability range of fuel-air mixtures. The lowest temperature at which a flammable fuel-air mixture can be formed, based upon the vapor pressure of the fuel at atmospheric pressure, is the flash point of that fuel-air mixture. Within the flammability range of a fuel-air mixture, at temperatures exceeding the flash point of the fuel-air mixture, auto-ignition of the fuel vapor occurs. Auto-ignition generally occurs at or slightly above the stoichiometric fuel-air mixture composition [9, 10]. The time interval between the mixing of the fuel-air mixture such that it is combustible and the auto-ignition of that fuel-air mixture is known as the auto-ignition delay time.

One reason that flame stabilization is required in combustion systems is to prevent the flame front from moving upstream from the combustion zone toward the source of fuel; a flashback [11, 12]. During a flashback event, the heat of combustion moves upstream and may damage numerous structures within the fuel and air mixing region of the combustor [11, 12]. Flashback may occur due to auto-ignition of a fuel-air mixture caused by a residence time of the fuel-air mixture in a region upstream of the combustion zone that exceeds the auto-ignition delay time of that fuel-air mixture at the temperature and pressure of that region.

Flame stabilization also is dependent upon speed of the fuel-air mixture entering the combustion zone where propagation of the flame is desired [13, 14]. A sufficiently low velocity must be retained in the region where the flame is desired in order to sustain the flame. A region of low velocity in which a flame can be sustained can be achieved by causing recirculation of a portion of the fuel-air mixture already burned thereby providing a source of ignition to the fuel-air mixture entering the combustion zone [13, 14]. However, the fuel-air mixture flow pattern, including any recirculation, is critical to achieving flame stability.

One method known for causing recirculation is the placement of a bluff body in the flow path of the fuel-air mixture within the combustion zone [15, 16]. A bluff body typically defines a leading edge and a trailing edge, and separation of a mixture passing over the bluff body occurs at the trailing edge of the bluff body thereby forming a wake downstream of the trailing edge [15, 16]. The velocity of the fuel-air mixture in the wake region is much lower than the velocity of the fuel-air mixture flowing in the main stream around the bluff body thereby supporting recirculation.

This study relates to the essential characteristics of catalytically stabilized combustion in a micro-scale system with a heat-recirculating structure. Numerical simulations are conducted to gain insights into system performance and to determine what changes can be made to improve its robustness and stability. Detailed kinetics are used for modelling the system in computational fluid dynamics. Methods of applying a heat-recirculating structure to the channel walls are employed, which may be utilized with presently existing designs of micro-scale combustion systems. The factors affecting combustion stability are determined for the system. The objective of this study is to investigate the essential characteristics of catalytically stabilized combustion in a micro-scale heat-recirculating system so as to gain a greater understanding of the mechanisms of flame stabilization. Particular focus is placed on determining essential factors for design considerations of the system with improved flame stability and combustion

characteristics so that the system operates more efficiently.

2. Computational details

Computational fluid dynamics is the analysis and prediction of fluid flows and heat transfer using a computer model [17, 18]. It may be used to predict the flows of fluids through a heat exchanger, or into the cylinder head of a diesel engine, or through a valve or a mixing vessel for example [19, 20]. The first stage involves constructing a numerical model of the structure around or through which the flows are occurring, this being similar to the process of computer aided design. It is also necessary to provide to the numerical model the nature of the fluid flow as it enters the structure. The second stage is to perform the computational fluid dynamics modelling for that structure and that input flow, this typically being performed in an iterative manner. The final stage is to convert the resulting flow information into an output form, for example a graphical representation showing the flow paths. Highly sophisticated software is now available for performing these activities, which enables a skilled user to model fluid flows and heat transfer in or around any conceivable structure.

The system configured to combust propane is illustrated schematically in Figure 1 with a heat-recirculating structure. The system comprises a concentric annular channel, wherein the concentric annular channel further comprises an inner annular channel and an outer annular channel. A platinum catalyst is deposited only upon the interior surface of the inner channel, and the wall of the outer channel is chemically inert and catalytically inactive. The reactant stream flows through the catalytically-coated inner channel and the product stream flows out of the outer non-catalytic channel. Fuel is present for combustion in both the catalytic and non-catalytic channels. The concentrically arranged annular channel is 5.0 mm in inner channel length, 5.6 mm in outer channel length, 0.8 mm in innermost diameter, 2.6 mm in outermost diameter, 0.1 mm in catalyst layer thickness, and 0.2 mm in wall thickness, unless otherwise stated. The system can have any dimension unless restricted by design requirements. All the walls have the same thickness. The spacing between the inner channel and the outer channel is 0.4 mm and remains constant. One of the potential problems associated with the system, as with all micro-scale combustion systems, continues to be combustion stability. The scale of the system is on the order of sub-millimeters, which is much smaller than the quenching distance of the combustible mixture in the absence of a catalyst. The quenching distance defines a critical dimension under which propagation of the propane flame is not possible. The quenching distance is approximately 2.5 mm, at which combustion cannot be sustained in the absence of a catalyst.

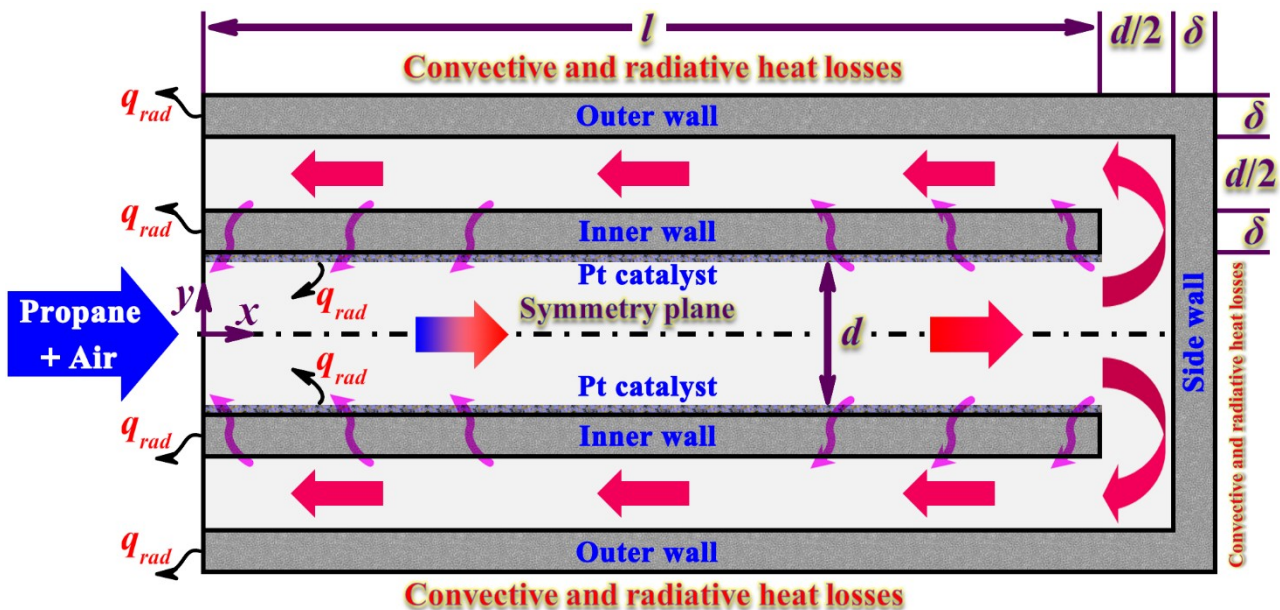


Figure 1. Schematic representation of the heat-recirculating continuous flow reactor for improved flame stabilization and energy efficiency. The direction of fluid flow in the system is indicated by arrows.

To gain a better understanding of the system, computational fluid dynamics simulations for propane-air combustion over a catalyst are performed. The insights gained from homogeneous combustion are not necessarily applicable to the catalytic systems studied in this work. For example, temperatures in gas-phase combustion are too high in comparison to those in catalytic combustion [21, 22]. Furthermore, while gaseous radicals are typically quenched on walls, causing flame extinction, catalysts serve mainly to form radicals that drive surface chemistry [23, 24]. Heat transfer is also different. For gaseous micro-burners, heat transfer of the heat generated in the gas phase to the walls can be slow in comparison to the chemistry time scale [25, 26]. On the other hand, the heat is liberated on the wall in catalytic microreactors, accelerating heat transfer within the walls [27, 28]. As a result of such differences, a model incorporating catalytic combustion is developed.

The specific heat, viscosity, and thermal conductivity are calculated using a mass fraction weighted average of the species properties. The species-specific heats are computed using a piecewise polynomial fit of the temperature. The species viscosities and thermal conductivity are determined from kinetic theory. Multicomponent diffusion is considered in this system, where the binary diffusion coefficients are determined from kinetic theory. A one-step, irreversible, catalytic reaction mechanism is used to model the propane-air catalytic combustion chemistry. Nonuniform node spacing is employed in this work, with more nodes in the reaction zone. The number of nodes varies depending on dimensions. Meshes in excess of 200,000 nodes are utilized for the largest dimensions. Typical wall node spacing is 50 microns in the axial direction and 20 microns in the transverse direction, where the temperature does not vary. Only a few nodes are placed in the transverse direction within the wall. However, as the mesh is nonuniform, these are just representative values.

Detailed chemistry is included in the model. Detailed chemical mechanisms are playing an increasingly important role in developing chemical kinetics models for combustion. Detailed chemical mechanisms are incorporated into the reacting flow for the system. The homogeneous combustion is modeled with the detailed chemical mechanism, GRI-MECH 3.0, in CHEMKIN format. Additionally, detailed heterogeneous chemistry in SURFACE-CHEMKIN format is also included in the model. The rates of the elementary reactions involved in the combustion process are determined by Arrhenius kinetic expressions. Numerical simulations with the detailed chemical mechanism are typically computationally expensive. The detailed chemical mechanism is invariably stiff and therefore its numerical integration is computationally costly.

The conservation equations were solved implicitly with a two-dimensional steady-state segregated solver using an under-relaxation method. The segregated solver first solves the momentum equation, then the continuity equation, and then updates the pressure and mass flow rate. The pressure is discretized using a Standard method. The pressure-velocity coupling is discretized using the SIMPLE method. The momentum, species, and energy equations are discretized using a two-order upwind approximation. The conservation equations are then checked for convergence. Convergence is determined from the residuals of the conservation equations as well as the difference between subsequent iterations of the solution. When parallel processing is used, the message passing interface is used to transmit information between nodes. In order to achieve convergence as well as compute extinction points, natural parameter continuation is implemented. The calculation time of each computational fluid dynamics simulation varies between several hours and several days, depending on the difficulty of the problem. The complex physicochemical processes involved in the system can require extensive computing resources. The computational fluid dynamics calculations may take days

in order to arrive at a reasonably accurate solution, using fine grids of the system, due to the time-consuming nature of the model.

3. Model validation

Validation of the model must be conducted prior to performing the computation. To estimate whether the model describes the system accurately or not, the model is compared with the experimental data under identical conditions. The catalyst surface temperature distribution measured by means of thermocouples is specified as the interfacial energy boundary conditions. The concentration profiles of typical species after onset of homogeneous combustion are presented in Figure 2 under different conditions, which are predicted by the model using computational fluid dynamics and determined from optical measurements using a planar-laser-induced-fluorescence detection system. The catalyst can facilitate ease of ignition under circumstances where ignition could not occur in normal conditions. The term ignition means the very onset of combustion or start of combustion. Along the fluid centerline, there is a sharp rise in the concentration of hydroxyl radicals, which indicates the onset of homogeneous combustion, as predicted by the model accurately. The model is therefore in reasonable agreement with the experimental measurements.

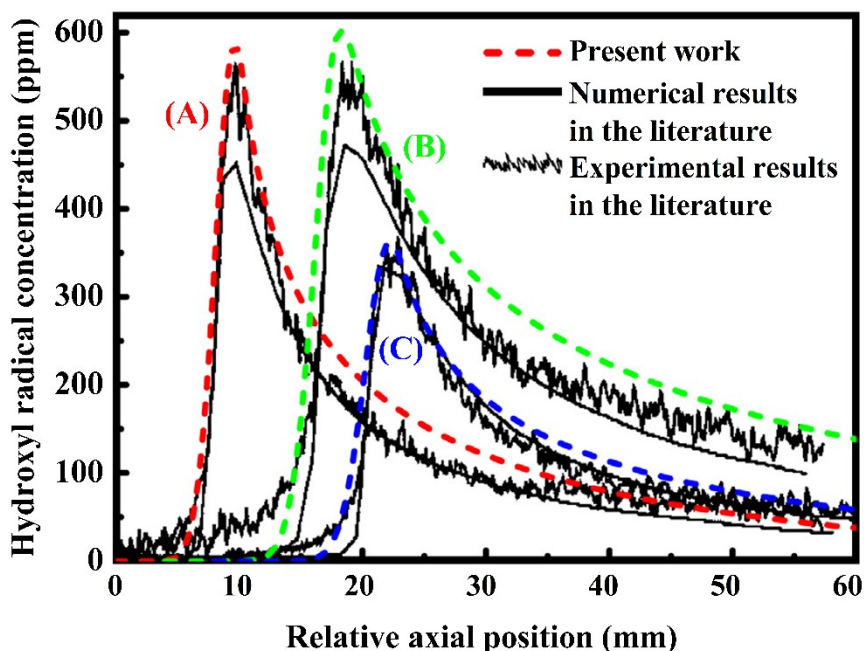


Figure 2. Hydroxyl radical concentrations along the centerline of the channel after onset of homogeneous combustion in the gas phase in different cases. The experimental data and numerical results obtained for the cases (a), (b), and (c) are incorporated herein. It is worth noting that the hydroxyl radical concentration profiles predicted by the model are shifted axially to match the measured peak hydroxyl radical locations.

4. Results and discussion

To understand the catalytically stabilized combustion process, the effect of temperature on the rate of reaction is evaluated. Accordingly, temperature boundary conditions are used to define the thermal properties at the boundaries between the gas phase and the solid phase. Specifically, a fixed temperature condition is applied at the walls of the channels.

A plot of the rate of reaction against the temperature of the catalyst is represented in Figure 3 for the system. The temperature of the catalyst is related closely to catalyst light-off, and consequently excessively low temperatures will cause difficulties in catalyst light-off. Initially, as the temperature of the catalyst is raised in the system, the rate of reaction also increases, as indicated in Figure 3 by the kinetic region A. The rate of reaction has an exponential dependence upon temperature [29, 30]. The

system operates within a transition region with further increasing the temperature of the catalyst. In the transition region, the factors that influence the rate of reaction shift from kinetics to mass transfer, as indicated in Figure 3 by the kinetic region B. When the rate of reaction is increased to such an extent that the rate of the heterogeneous catalytic surface oxidation reaction is much faster than the rate of transport of the gas-phase reactants onto the catalytically active surface, the surface reaction is almost entirely diffusion controlled, and the rate of reaction is substantially constant thereafter regardless of the level of the catalyst temperature. In this case, the system operates in the mass-transfer controlled regime [31, 32], as indicated in Figure 3 by the kinetic region C. As the catalyst temperature is raised substantially into the diffusion-controlled region, the rate of reaction begins to increase exponentially again with the temperature of the catalyst, as indicated in Figure 3 by the kinetic region D. This exists an apparent contradiction between the laws of mass transfer kinetics and catalytic technology.

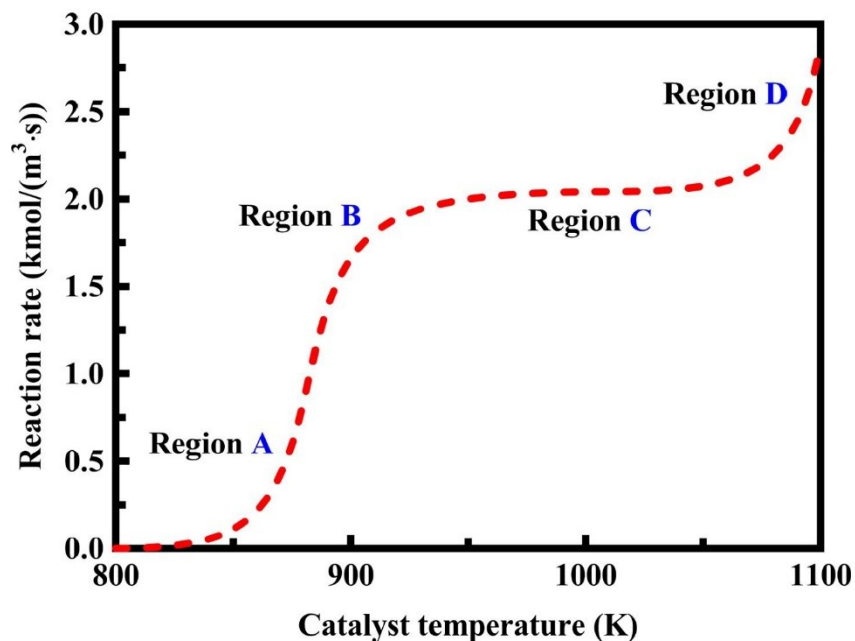


Figure 3. Rate of reaction as a function of the temperature of the catalyst. A fixed temperature condition is applied at the walls of the channels. The equivalence ratio of the mixture is 0.8, and the flow velocity is 9.0 m/s at the flow inlet.

The above apparent contradictory problem can be addressed in view of the following fact: the temperature of both the catalytically active surface and its adjacent fluid region has been raised to such a high level that the homogeneous combustion reaction takes place in the gas phase at rates significantly higher than those of the heterogeneous catalytic surface oxidation reaction. Under such circumstances, the temperature of the catalytically active surface is higher than the autoignition temperature of the mixture, as shown in Figure 3. The combustible gas ignites spontaneously in the fluid layer without transport into the catalyst layer. The fluid layer becomes thicker with the progress of combustion. The temperature of the total mixture can ultimately be raised to such a high level that the homogeneous combustion reaction takes place in the entire fluid stream. Once such a stage is reached within the system, the thermal flame combustion reaction continues even without further contact of the gaseous reactants with the catalytically active surface when the fluid passes through the homogeneous reaction region. Under such circumstances, the total reaction can take place at rates significantly higher than those of the surface reaction under diffusion-controlled conditions. Consequently, the catalytically stabilized combustion system is essentially free of mass transfer limitations.

The surface reaction rate profiles along the length of the inner channel are shown in Figure 4 under different flow velocity conditions. The rate of the surface reaction is determined from the average rate over the cross-section of the catalytically-active layer. The rate of the surface reaction

increases with increasing the flow velocity at the flow inlet, and therefore the catalyst employed in the exothermic reaction can provide quite satisfactory catalytic performance for the system. Initially, as the flow velocity increases at the flow inlet, the rate of the surface reaction also increases. As the flow velocity of the reactants is increased further through the catalyst layer, the rate of the surface reaction falls within the transition region. At high flow velocity of the reactants, the system operates in the mass-transfer controlled regime, and the rate of the surface reaction levels off regardless of further increases in flow velocity, as shown in Figure 4. High flow velocities of the reactants will enable mass transfer control of the surface reaction. The surface reaction is therefore considered to be diffusion-controlled. The surface reaction occurs essentially at a rate equal to the rate of transport of the gaseous reactants onto the catalytically active surface. Therefore, the rate of the surface reaction is limited or controlled primarily by the extent of the contact between the reactants and the surface, which means the extent of transport of the reactants in the gas phase onto contact the surface. With the increase of flow velocity, however, the distance required for the reactants to diffuse through the stream and contact the catalytically active surface is essentially unchanged, since the flow is laminar in nature. A further increase in flow velocity may therefore be disadvantageous, since a blowout of the flame can occur. In the mass-transfer controlled regime, the surface reaction is limited by diffusion control.

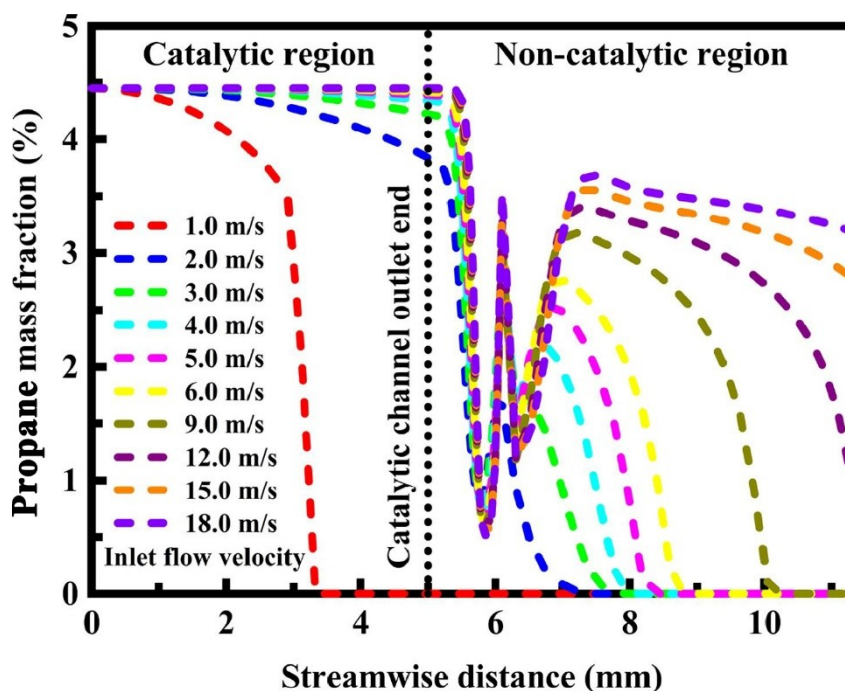


Figure 4. Surface reaction rate profiles along the length of the inner channel under different flow velocity conditions. The equivalence ratio of the mixture is 0.8, and the exterior heat loss coefficient is $20 \text{ W}/(\text{m}^2 \cdot \text{K})$. The thermal conductivity of the interior wall is $200 \text{ W}/(\text{m} \cdot \text{K})$, and the thermal conductivity of the exterior wall is $20 \text{ W}/(\text{m} \cdot \text{K})$.

The two-dimensional contour plots of temperature at different streamwise distances are presented in Figure 5 for the system under different flow velocity conditions. For the catalytic inner channel, the difference in temperature is small between different flow velocities. For the chemically inert outer channel, however, this difference is significant between different flow velocities. These results obtained under varying flow conditions are consistent with those obtained for propane concentration in the system. Interestingly, the maximum temperature of the catalytically stabilized combustion system can reach beyond the adiabatic flame temperature. When the flow velocity of the reactants is 18.0 m/s at the flow inlet, however, catalytically stabilized thermal combustion takes place at much lower temperatures than conventional gas-phase combustion under adiabatic conditions. This is caused by incomplete homogeneous combustion in the gas phase due to the substantially reduced residence time,

as discussed above. At moderate flow velocities, the total residence time is sufficiently long in the system relative to the total channel length. At the specified equivalence ratio, the system can operate at a maximum temperature well above the theoretical temperature produced by a flame that loses no heat, as illustrated in Figure 5. At high flow velocities, long residence times are needed for combustion completion in the gas phase, downstream of the catalyst structure.

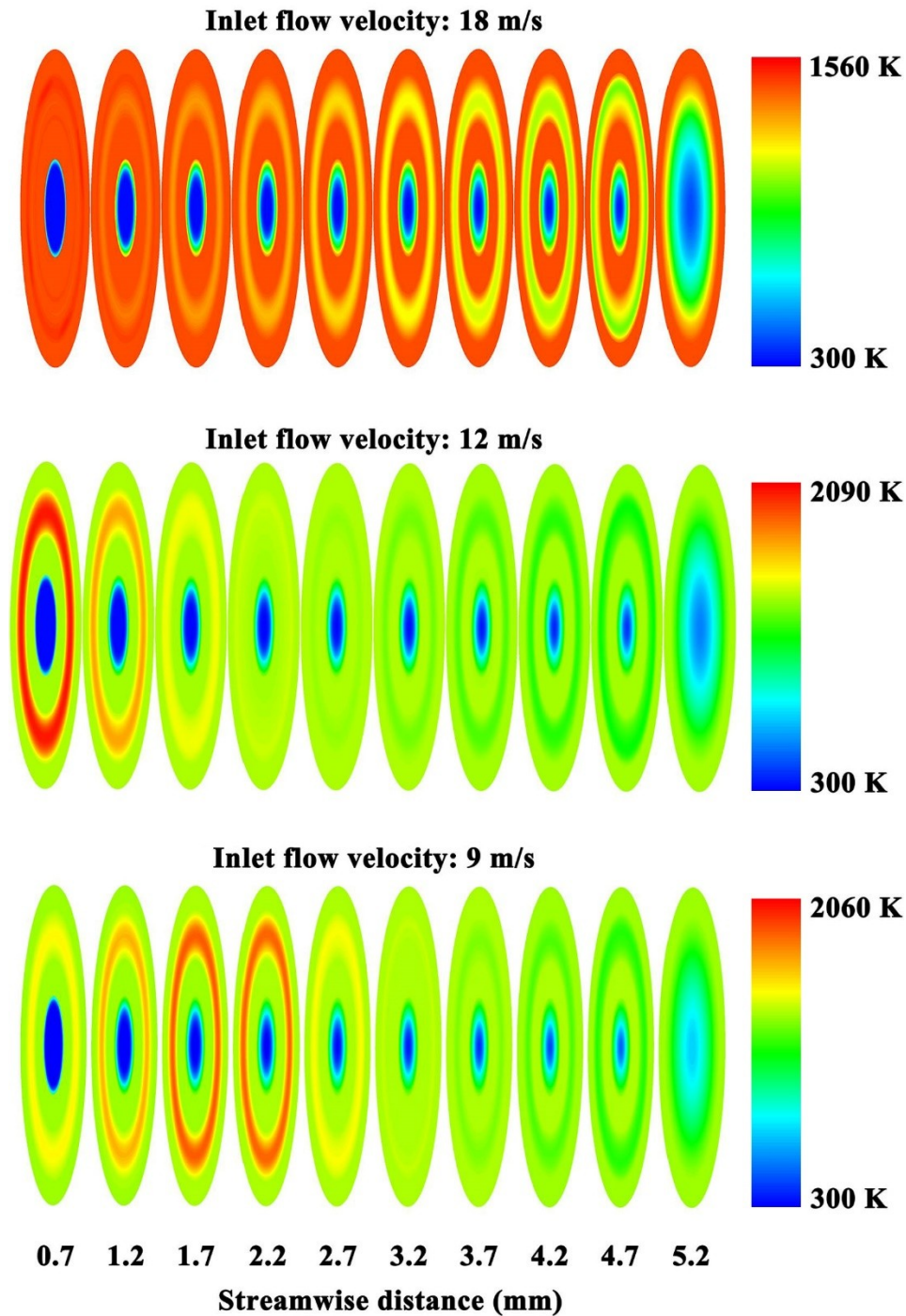


Figure 5. Contour plots of temperature at different streamwise distances for the system under different flow velocity conditions. The equivalence ratio of the mixture is 0.8, and the exterior heat loss coefficient is $20 \text{ W}/(\text{m}^2\cdot\text{K})$. The thermal conductivity of the interior wall is $200 \text{ W}/(\text{m}\cdot\text{K})$, and the thermal conductivity of the exterior wall is $20 \text{ W}/(\text{m}\cdot\text{K})$.

In order to provide the maximum flow velocity limits for preventing blowout and optimizing operation, the effects of wall thermal conductivity and exterior heat loss coefficient on the catalytically stabilized combustion characteristics are investigated. The contour map of the critical flow velocity determined by a blowout limit is presented in Figure 6 under different thermal conditions. The critical

flow velocity to prevent blowout is much higher under adiabatic conditions. Significant heat loss is not conducive to flame stabilization. The solid walls having a high thermal conductivity may allow effective operations of the system to be performed at high flow velocities. At the other extreme, the solid walls having a low thermal conductivity will lead to minimum allowable flow velocities, as shown in Figure 6. However, the system requires much less heat recirculation and will be more robust against the surrounding conditions, thereby insulating the outer wall against heat loss to the ambient environment. When designing such a catalytically stabilized combustion system, it will be important to select an appropriate thermal conductivity range for the solid walls so that high flame stability can be achieved. It is preferred that the solid material is highly conductive [33, 34], thereby achieving desired high power for the system [35, 36]. At the other extreme, the solid material is preferred to be highly insulating when low power is desired. The above criteria are determined based upon a particular application, for example, combustion stability. When designing the system, however, other properties must also be considered for the solid material.

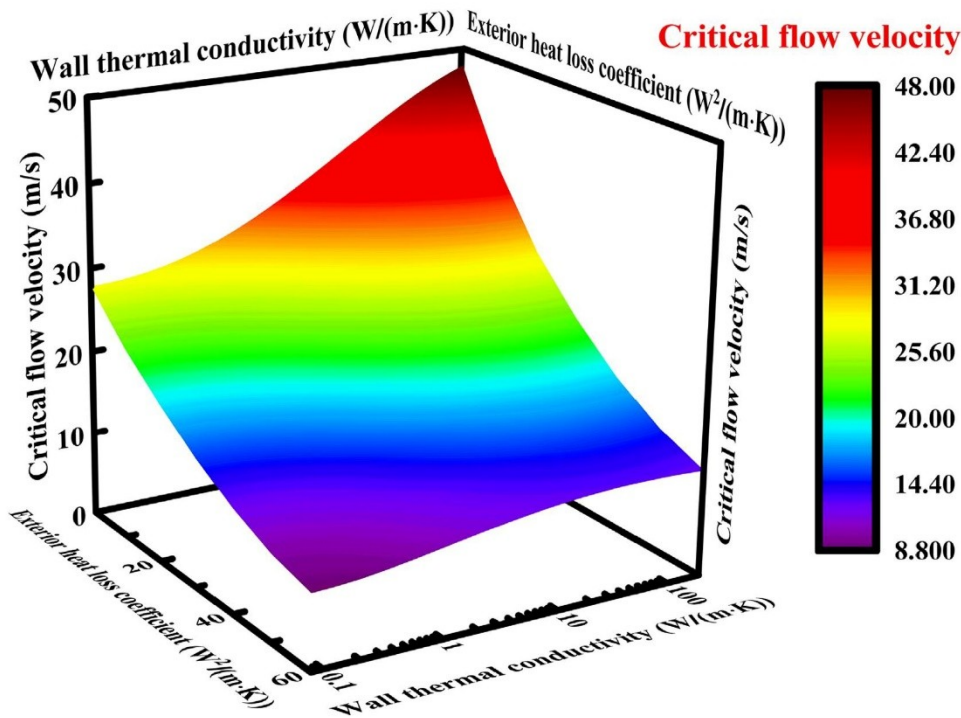


Figure 6. Contour map of the critical flow velocity determined by a blowout limit for the system under different thermal conditions. The equivalence ratio of the mixture is 0.8, and all the walls have the same thermal conductivity.

Flame stabilization is a common problem in micro-scale combustion systems [37, 38]. Flame stabilization is dependent upon the flow velocity of the fuel-air mixture entering the combustion region in which propagation of the flame is desired [39, 40]. The flame will propagate in the gas phase only when certain flow conditions prevail.

The stability diagram for catalytically stabilized combustion in the system is presented in Figure 7 in terms of the critical flow velocity. The laminar flame speed determined by experiments [41, 42] is plotted as a dashed horizontal line. A sufficiently low flow velocity must be retained in the region in which a stable and therefore efficient flame is desired in order to sustain the flame, thereby avoiding any issue from blowout events due to insufficient residence time [43, 44], as presented in Figure 7 by the upper curve. Similarly, a sufficiently high flow velocity of the fluid must be retained within the system in order to sustain the flame, thereby avoiding any issue from extinction events due to insufficient heat generated, as presented in Figure 7 by the lower curve. Stable operation of the continuous combustion system is limited to a relatively wide flow regime, and the shaded region

indicated in Figure 7 allows catalytically stabilized combustion. This means that self-sustained combustion is achieved only if the flow velocity of the fluid lies within the lower and upper bounds. Outside the bounds of the critical flow velocity, catalytically stabilized combustion is impossible. The system enables catalytically stabilized combustion to occur downstream of the catalyst structure at a flow velocity higher than the laminar flame speed without any issue from blowout events [45, 46], but has difficulty maintaining a stable flame at very high or low flow velocities [47, 48]. According to the computational fluid dynamics analysis, the flow velocity is critical to achieving flame stability. Under the conditions specified, the maximum allowable flow velocity does exceed the laminar flame speed, as indicated in Figure 7. Heat recirculation is obtained by the structure design and homogeneous combustion is initiated by free radicals, thereby providing improved stability for the system.

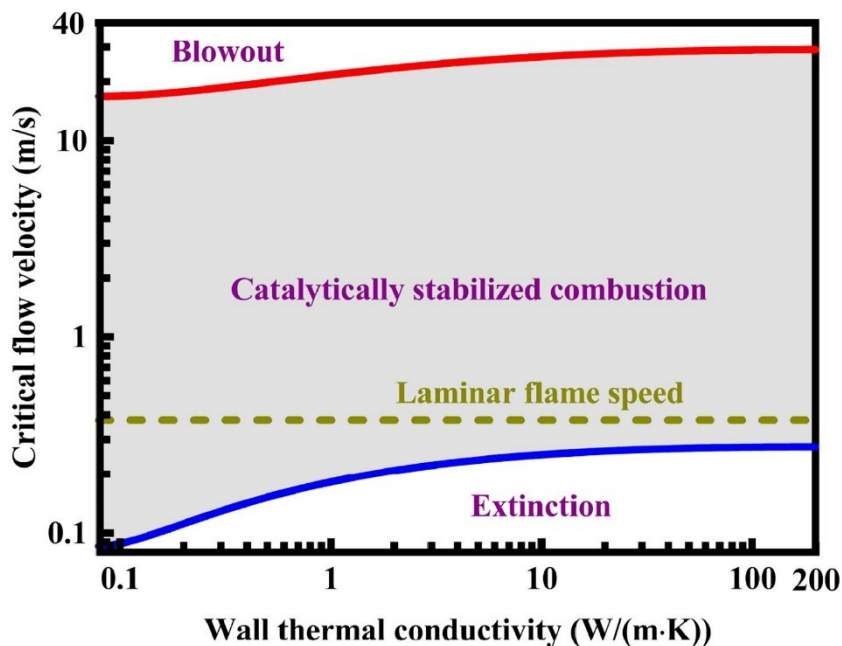


Figure 7. Stability diagram for catalytically stabilized combustion in the heat-recirculating continuous flow reactor in terms of the critical flow velocity. The equivalence ratio of the mixture is 0.8, and the exterior heat loss coefficient is $20 \text{ W}/(\text{m}^2 \cdot \text{K})$. All the walls have the same thermal conductivity. The laminar flame speed determined by experiments is plotted as a dashed horizontal line. The shaded region allows catalytically stabilized combustion. Stable operation of the system is limited to a relatively wide flow regime: the upper curve represents blowout due to insufficient residence time, whereas the lower curve represents extinction due to insufficient heat generated.

The propane mass fraction profiles along the fluid centerline are shown in Figure 8 under different flow velocity conditions. At high flow velocities at the flow inlet, the system operates in the mass-transfer controlled regime, and therefore there is no significant difference in propane concentration at the outlet end of the catalyst structure, as shown in Figure 8. In the non-catalytic region, however, there is significant difference in propane concentration between different flow velocities, as shown in Figure 8, even if the system operates in the mass transfer-controlled regime. Homogeneous combustion in the gas phase is no longer limited by diffusion control. At low flow velocities at the flow inlet, the system is essentially free of mass transfer limitations, followed by complete homogeneous combustion of the fuel at the outlet end of the system, as shown in Figure 8. At high flow velocities at the flow inlet, the homogeneous combustion is incomplete in the gas phase due to the substantially reduced residence time. It is essential to have sufficient total residence time to allow achievement of the required conversion level, for example, essentially complete combustion of the fuel. In order for flame holding to occur in the gas phase, fuel and air must be provided in a low-to-moderate velocity region to reside. The counter-current flow of the fluid around the channel corners would give rise to instabilities in

propane concentration, enthalpy, and flow velocity. As a result, the propane concentration along the fluid centerline varies significantly in the corner regions, as shown in Figure 8. Clearly, the heat and mass transfer within the system can be improved with counter-current exchange.

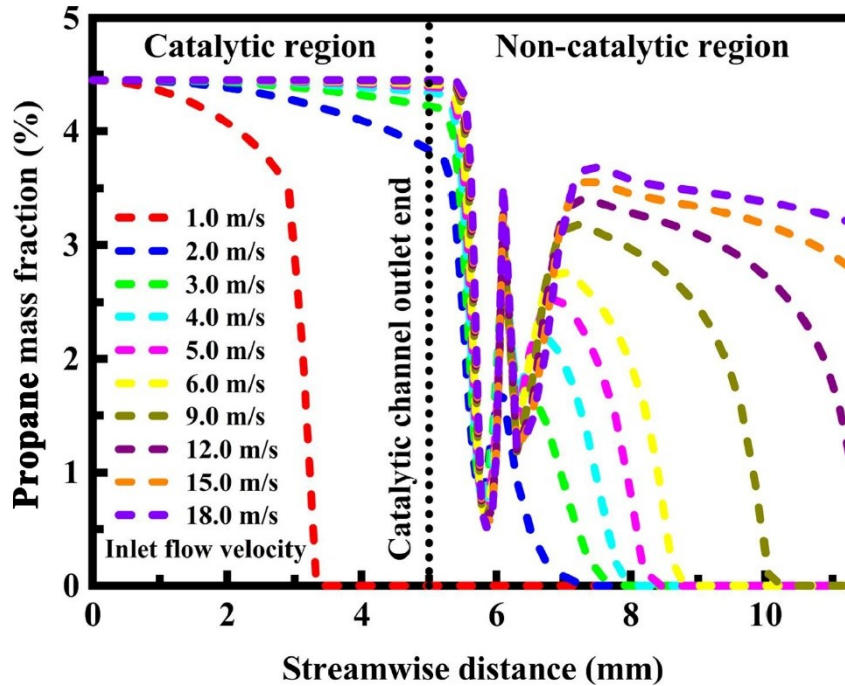


Figure 8. Propane mass fraction profiles along the fluid centerline under different flow velocity conditions. The equivalence ratio of the mixture is 0.8, and the exterior heat loss coefficient is $20 \text{ W}/(\text{m}^2 \cdot \text{K})$. The thermal conductivity of the interior wall is $200 \text{ W}/(\text{m} \cdot \text{K})$, and the thermal conductivity of the exterior wall is $20 \text{ W}/(\text{m} \cdot \text{K})$.

5. Conclusions

This study is focused mainly upon the essential combustion characteristics of propane-air mixtures in heat-recirculating continuous flow reactors. Numerical simulations are performed to gain a greater understanding of the mechanisms of flame stabilization. The essential factors affecting flame stability and combustion characteristics are determined in order to obtain design insights. The main conclusions are summarized as follows:

- Stable operation of the system is limited to a relatively wide flow regime, and the flow velocity is critical to achieving flame stability. There is an optimum wall thermal conductivity for the system in terms of flame stability. For moderate wall thermal conductivities, the system will be most robust against the surrounding conditions. Thermally insulative materials are not conducive to flame stabilization due to the lack of heat recirculation. Thermally conductive materials are also not conducive to flame stabilization due to a significant loss of heat to the surroundings.
- Blowout shifts homogeneous combustion downstream significantly without substantially reducing the reaction rate. This has important implications for understanding how to design the system with increased robustness and stability.
- The system represents a unique approach to combustion that incorporates the best features of both catalytic combustion method and thermal flame method. Efficient, rapid thermal combustion can occur, resulting from the injection of free radicals and heat produced by the catalytic reaction.
- The flow velocity, wall thermal conductivity, equivalence ratio, exterior heat losses are important factors affecting the stability of the combustion process.
- The catalytically stabilized combustion system can surmount mass transfer limitations. Additionally, stability of the combustion process can be improved by inducing heat recirculation.

Furthermore, excess enthalpy combustion can occur, and the maximum temperature can reach beyond the adiabatic flame temperature.

References

- [1] Y.S. Seo, S.J. Cho, S.K. Kang, and H.D. Shin. Experimental and numerical studies on combustion characteristics of a catalytically stabilized combustor. *Catalysis Today*, Volume 59, Issues 1-2, 2000, Pages 75-86.
- [2] J. Mantzaras, C. Appel, P. Benz, and U. Dogwiler. Numerical modelling of turbulent catalytically stabilized channel flow combustion. *Catalysis Today*, Volume 59, Issues 1-2, 2000, Pages 3-17.
- [3] D. Lozinski, J. Buckmaster, and P. Ronney. Absolute flammability limits and flame-balls. *Combustion and Flame*, Volume 97, Issues 3-4, 1994, Pages 301-316.
- [4] Y.N. Shebeko, S.G. Tsarichenko, A.Y. Korolchenko, A.V. Trunev, V.Y. Navzenya, S.N. Papkov, and A.A. Zaitzev. Burning velocities and flammability limits of gaseous mixtures at elevated temperatures and pressures. *Combustion and Flame*, Volume 102, Issue 4, 1995, Pages 427-437.
- [5] C.T. Cloney, R.C. Ripley, M.J. Pegg, and P.R. Amyotte. Laminar combustion regimes for hybrid mixtures of coal dust with methane gas below the gas lower flammability limit. *Combustion and Flame*, Volume 198, 2018, Pages 14-23.
- [6] H. Ohtani, S. Horiguchi, Y. Urano, M. Iwasaka, K. Tokuhashi, and S. Kondo. Flammability limits of arsine and phosphine. *Combustion and Flame*, Volume 76, Issues 3-4, 1989, Pages 307-310.
- [7] A. Bertolino, A. Stagni, A. Cuoci, T. Faravelli, A. Parente, and A. Frassoldati. Prediction of flammable range for pure fuels and mixtures using detailed kinetics. *Combustion and Flame*, Volume 207, 2019, Pages 120-133.
- [8] R.Y. Tam and G.S.S. Ludford. The lean flammability limit: A four-step model. *Combustion and Flame*, Volume 72, Issue 1, 1988, Pages 35-43.
- [9] Z.H. Chen and S.H. Sohrab. Flammability limit and limit-temperature of counterflow lean methane-air flames. *Combustion and Flame*, Volume 102, Issues 1-2, 1995, Pages 193-199.
- [10] N. Peters and M.D. Smooke. Fluid dynamic-chemical interactions at the lean flammability limit. *Combustion and Flame*, Volume 60, Issue 2, 1985, Pages 171-182.
- [11] S.J. Lim, A.K. Alwahaibi, F.L. Dryer, and S.H. Won. Impacts of preferential vaporization on flashback behaviors of multi-component liquid fuels. *Combustion and Flame*, Volume 245, 2022, Article Number: 112300.
- [12] F.A. Lammers and L.P.H. de Goey. A numerical study of flash back of laminar premixed flames in ceramic-foam surface burners. *Combustion and Flame*, Volume 133, Issues 1-2, 2003, Pages 47-61.
- [13] F.H. Vance, A. Scholtissek, P. de Goey, J. van Oijen, and C. Hasse. Dynamic stabilization of a hydrogen premixed flame in a narrow channel. *Combustion and Flame*, Volume 248, 2023, Article Number: 112560.
- [14] F.H. Vance, Y. Shoshin, L.P.H. de Goey, and J.A. van Oijen. An investigation into flashback and blow-off for premixed flames stabilized without a recirculation vortex. *Combustion and Flame*, Volume 235, 2022, Article Number: 111690.
- [15] M.K. Geikie, C.J. Rising, A.J. Morales, and K.A. Ahmed. Turbulent flame-vortex dynamics of bluff-body premixed flames. *Combustion and Flame*, Volume 223, 2021, Pages 28-41.
- [16] K.S. Kedia and A.F. Ghoniem. The anchoring mechanism of a bluff-body stabilized laminar premixed flame. *Combustion and Flame*, Volume 161, Issue 9, 2014, Pages 2327-2339.
- [17] C.R. Kaplan, S.W. Baek, E.S. Oran, and J.L. Ellzey. Dynamics of a strongly radiating unsteady ethylene jet diffusion flame. *Combustion and Flame*, Volume 96, Issues 1-2, 1994, Pages 1-21.
- [18] P.A. Gillis and P.J. Smith. An evaluation of three-dimensional computational combustion and fluid-

- dynamics for industrial furnace geometries. *Symposium (International) on Combustion*, Volume 23, Issue 1, 1991, Pages 981-991.
- [19] H.A. Dwyer and B.R. Sanders. Detailed computation of unsteady droplet dynamics. *Symposium (International) on Combustion*, Volume 20, Issue 1, 1985, Pages 1743-1749.
- [20] G. Patnaik and K. Kailasanath. A computational study of local quenching in flame-vortex interactions with radiative losses. *Symposium (International) on Combustion*, Volume 27, Issue 1, 1998, Pages 711-717.
- [21] G.J. Griffin and D.G. Wood. Non-adiabatic catalytic combustion at a fin surface involving heat extraction from the fin edge. *Combustion and Flame*, Volume 125, Issue 4, 2001, Pages 1230-1238.
- [22] K. Maruta, K. Takeda, J. Ahn, K. Borer, L. Sitzki, P.D. Ronney, and O. Deutschmann. Extinction limits of catalytic combustion in microchannels. *Proceedings of the Combustion Institute*, Volume 29, Issue 1, 2002, Pages 957-963.
- [23] A. James, J. Brindley, and A.C. McIntosh. Stability of multiple steady states of catalytic combustion. *Combustion and Flame*, Volume 130, Issues 1-2, 2002, Pages 137-146.
- [24] T. Kim and M.S. Wooldridge. Burning velocities in catalytically assisted self-propagating high-temperature combustion synthesis systems. *Combustion and Flame*, Volume 125, Issues 1-2, 2001, Pages 965-973.
- [25] M.R. Dongworth and A. Melvin. Diffusive catalytic combustion. *Symposium (International) on Combustion*, Volume 16, Issue 1, 1977, Pages 255-264.
- [26] J. Wolfrum. Lasers in combustion: From basic theory to practical devices. *Symposium (International) on Combustion*, Volume 27, Issue 1, 1998, Pages 1-41.
- [27] J. Mantzaras and C. Appel. Effects of finite rate heterogeneous kinetics on homogeneous ignition in catalytically stabilized channel flow combustion. *Combustion and Flame*, Volume 130, Issue 4, 2002, Pages 336-351.
- [28] S.L. Hung, A. Barresi and L.D. Pfefferle. Flow tube reactor studies of catalytically stabilized combustion of methyl chloride. *Symposium (International) on Combustion*, Volume 23, Issue 1, 1991, Pages 909-915.
- [29] J.E. Rehm and P.H. Paul. Reaction rate imaging. *Proceedings of the Combustion Institute*, Volume 28, Issue 2, 2000, Pages 1775-1782.
- [30] B.M. Cetegen and W.A. Sirignano. Study of molecular mixing and a finite rate chemical reaction in a mixing layer. *Symposium (International) on Combustion*, Volume 22, Issue 1, 1989, Pages 489-494.
- [31] F. Takahashi, W.J. Schmoll, and V.R. Katta. Attachment mechanisms of diffusion flames. *Symposium (International) on Combustion*, Volume 27, Issue 1, 1998, Pages 675-684.
- [32] M. Nishioka, Y. Takemoto, H. Yamashita, and T. Takeno. Effects of multi-dimensionality on a diffusion flame. *Symposium (International) on Combustion*, Volume 26, Issue 1, 1996, Pages 1071-1077.
- [33] M.V. Heitor and J.H. Whitelaw. Velocity, temperature, and species characteristics of the flow in a gas-turbine combustor. *Combustion and Flame*, Volume 64, Issue 1, 1986, Pages 1-32.
- [34] J.A. Clark. Measured and predicted soot profiles in a gas turbine combustor. *Combustion and Flame*, Volume 48, 1982, Pages 121-133.
- [35] J.A. Senecal and C.W. Shipman. Mass transfer and reaction rates in a ducted propane-air diffusion flame. *Symposium (International) on Combustion*, Volume 17, Issue 1, 1979, Pages 355-362.
- [36] K.H. Luo and K.N.C. Bray. Combustion-induced pressure effects in supersonic diffusion flames. *Symposium (International) on Combustion*, Volume 27, Issue 2, 1998, Pages 2165-2171.
- [37] J.M. Beér. Combustion technology developments in power generation in response to environmental challenges. *Progress in Energy and Combustion Science*, Volume 26, Issues 4-6, 2000, Pages 301-

- [38] P.O. Hedman and D.L. Warren. Turbulent velocity and temperature measurements from a gas-fueled technology combustor with a practical fuel injector. *Combustion and Flame*, Volume 100, Issues 1- 2, 1995, Pages 185-192.
- [39] I.R. Gran, M.C. Melaaen, and B.F. Magnussen. Numerical simulation of local extinction effects in turbulent combustor flows of methane and air. *Symposium (International) on Combustion*, Volume 25, Issue 1, 1994, Pages 1283-1291.
- [40] W.C. Pfefferle and L.D. Pfefferle. Catalytically stabilized combustion. *Progress in Energy and Combustion Science*, Volume 12, Issue 1, 1986, Pages 25-41.
- [41] Y. Dong, C.M. Vagelopoulos, G.R. Spedding, and F.N. Egolfopoulos. Measurement of laminar flame speeds through digital particle image velocimetry: Mixtures of methane and ethane with hydrogen, oxygen, nitrogen, and helium. *Proceedings of the Combustion Institute*, Volume 29, Issue 2, 2002, Pages 1419-1426.
- [42] C.M. Vagelopoulos and F.N. Egolfopoulos. Direct experimental determination of laminar flame speeds. *Symposium (International) on Combustion*, Volume 27, Issue 1, 1998, Pages 513-519.
- [43] D. Han and M.G. Mungal. Observations on the transition from flame liftoff to flame blowout. *Proceedings of the Combustion Institute*, Volume 28, Issue 1, 2000, Pages 537-543.
- [44] W.M. Pitts. Importance of isothermal mixing processes to the understanding of lift-off and blowout of turbulent jet diffusion flames. *Combustion and Flame*, Volume 76, Issue 2, 1989, Pages 197-212.
- [45] D. Feikema, R.-H. Chen, and J.F. Driscoll. Blowout of nonpremixed flames: Maximum coaxial air velocities achievable, with and without swirl. *Combustion and Flame*, Volume 86, Issue 4, 1991, Pages 347-358.
- [46] G.A. Karim, I. Wierzba, and M. Hanna. The blowout limit of a jet diffusion flame in a coflowing stream of lean gaseous fuel-air mixtures. *Combustion and Flame*, Volume 57, Issue 3, 1984, Pages 283-288.
- [47] D. Feikema, R.-H. Chen, and J.F. Driscoll. Enhancement of flame blowout limits by the use of swirl. *Combustion and Flame*, Volume 80, Issue 2, 1990, Pages 183-195.
- [48] W.-P. Shih, J.G. Lee, and D.A. Santavicca. Stability and emissions characteristics of a lean premixed gas turbine combustor. *Symposium (International) on Combustion*, Volume 26, Issue 2, 1996, Pages 2771-2778.