EXPERIMENTAL APPARATUS AND MODELING FRAMEWORK FOR STUDYING COUNTER-FLOW LAMINAR FLAMES

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Abstract

Laboratory scale platform suitable for investigations on the structure of laminar diffusion and premixed flames in a counter-flow burner configuration is reported within this work. In particular, it is focused on design and setup of counter-flow burner apparatus specifically aimed at stabilization of laminar premixed cool flames. One-dimensional numerical simulations of dimethyl ether-air flames with detailed chemical kinetics and multi-component transport were carried out. More complex, three-dimensional, numerical simulations were performed assuming axially symmetric flow fields in realistic burner geometry, when addressing the effect of different nozzle shape on the flow-fields and corresponding flame structure.

Keywords: counter-flow burner, laminar flame, modeling.

1 Introduction

Physicochemical processes of reaction kinetics, thermodynamics and fluid flow including turbulence are strongly coupled in real flames [1]. Idealized systems including different burner configurations are utilized across the community of combustion modelers and experimentalists to study these phenomena [2]. Laminar flames are crucial for fundamental research and important from practical point of view as well (e.g. for application of the flamelet concept [3]). Assuming the case of stretched steady laminar flame stabilized in an opposed flow, complex chemistry-transport interactions can be investigated in more details employing both appropriate modeling tools and feasible experimental techniques.

Counter-flow burners are suitable for studying laminar non-premixed (diffusion) and premixed or partially premixed flames, their structure (temperature and speciation) as well as parameters of flame stability (extinction/ignition) and propagation [4, 5]. Following the formulation given in [6]: (I) double jet and (II) porous cylinder problems can be defined. In idealized case reaction zone is formed in the vicinity of the stagnation plane, which is perpendicular to flow direction of reactants, i.e. flat in case (I) or curved in case (II). It was discussed previously [7], that either plug-flow (Ia) or potential-flow (Ib) boundary condition needs to be assumed for optimal model representation of the former case. Therefore, an important issue arises concerning counter-flow burner design and setup, which is particularly addressed through this work.

2 Burner design and setup

Our counter-flow burner is designed according to Bundy et al. [8] following the conceptual work of Puri and Seshadri [9]. Initial aim related to this device was focused on the structure and dynamics of inhibited counter-flow non-premixed flames at low and moderate strain rate, which is of practical importance in the context of fire safety science. Our latest attempts are motivated by the recent progress of numerical simulations [10] and new experimental findings [11] regarding stabilization of low-temperature combustion (LTC) regime, i.e. so called cool flames in counter-flow configuration.
Following these investigators we proposed and realized the modified version of counter-flow burner which is depicted in the Figure 1. Such design is presumed to provide steady laminar cool flames enabling to study their structure. Burner apparatus is installed in measurement section of the experimental facility suitable for optical diagnostics in laminar flames and gaseous flows \[12, 13\]. Axis of the burner is aligned vertically to obtain symmetric shape of reaction zone at atmospheric pressure and normal gravity.

However, there is a lack of experimental evidence concerning flow-field characterization and behavior of the given burner setup under the conditions relevant for stabilization of cool flames. Moreover, an adaptation of the fuel inlet nozzle is anticipated here to eliminate the effect of flame curvature, which was observed previously \[8\]. State-of-the-art modeling tools involving detailed chemical kinetics were used in this work in order to accomplish a step targeted towards prediction-based experimental campaign.

### 3 Computation of laminar flame structure

Dimethyl ether (DME) was selected as a representative fuel for this study due to several reasons. Firstly, combustion characteristics of DME flames are of significant practical interest as it is considered as viable alternative fuel for transportation, heating and electricity generation. Further, according to recent observations, low-temperature oxidation mode of DME can be stabilized in counter-flow at atmospheric pressure \[11\]. This feature enables to investigate both high-temperature combustion (HTC) and LTC regimes in the given experimental configuration. Detailed chemistry of DME oxidation was investigated extensively in previous decade \[14\], thus validated chemical kinetic schemes with improved performance and reliability are available in the literature \[15\]. Finally, a model reduction to a skeletal DME oxidation scheme was reported by Pan et al. \[16\] and lately by Khare et al. \[17\]. Application of such reduced schemes is of paramount importance for performing computationally intensive simulations of chemically reacting flows in complex geometry.
3.1 One-dimensional model

The system of differential (governing) equations describing the counter-flow non-premixed flame in 1-D configuration [6] was solved employing the damped Newton method and time integration solution scheme as implemented in CANTERA software package (version 2.2). Plug flow boundary condition was specified on both sides in relevance to (Ia) case described above. Temperature profile was calculated based on the solution of an energy equation. Each numerical simulation with detailed chemical kinetic scheme was performed in several steps involving adaptive grid refinement method. Steady-state solution taking into account multi-component transport (including the effect of thermophoresis) was finally obtained.

3.2 Multi-dimensional model

A three-dimensional (3-D) rotational periodic model of the burner apparatus was generated. The computational domain and boundary conditions are shown in the Figure 2. Three inlet boundary conditions were included within the computational domain. Inlet 1 represents flow of DME/oxygen mixture. Inlet 2 represents cold nitrogen co-flow at the same temperature as a given flammable mixture and Inlet 3 corresponds to an opposed flow of heated nitrogen ($T = 675$ K). Boundary condition called Outlet 1 represents ambient pressure and Outlet 2 represents exhaust suction of combustion products. A steady-state solution of the particular simulation cases was obtained by using finite volume method. The FLUENT 18.2 software package was employed for 3-D numerical simulations as well as for post-processing of the modeling results. Computational grid containing about $360k$ cells was mainly composed of hexagonal elements. Convergence criteria for the governing equations of mass, momentum, energy and species conservation which were solved in combination with an ideal gas equation of state were set to $1 \times 10^{-6}$.

![Figure 2: Graphical representation of boundary conditions utilized for 3-D numerical simulations](image)
Whereas the Reynolds number characteristic for the counter-flowing jets is very low \((Re \approx 300)\) so the laminar model with SIMPLE algorithm and second order discretization schemes were employed. Temperature-dependent chemical reaction rate coefficients as well as thermodynamic and transport properties of all species were specified based on the data imported from CHEMKIN format files provided as supplementary material of [17]. The Laminar Finite-Rate chemistry model and Stiff Chemistry Solver were utilized to evaluate chemical reaction source terms for each computational timestep.

4 Results and discussion

In an initial stage of this work selection of reduced chemical kinetic scheme was performed based on 1-D modeling study. Experimental conditions corresponding to laser-based measurement of temperature and species concentrations in laminar counter-flow DME-air flames [18] were used for comparison of 1-D model performance with selected chemical kinetic schemes [15, 16, 17].

Figure 3: Temperature profiles (A) and mole fractions of molecular oxygen (B), hydroxyl radical (C) and formaldehyde (D) in a counter-flow non-premixed flame as predicted by 1-D model with different chemical kinetic schemes.
Results obtained with reduced scheme developed by Pan et al. [16] show lower reactivity on the fuel-lean side of a non-premixed flame when compared to prediction obtained with detailed DME oxidation scheme [15], see Figure 3. This behavior is accompanied by lower oxygen ($O_2$) consumption, underestimated peak flame temperature ($T_{\text{max}}$) and hydroxyl (OH) radical concentration. Moreover, position of OH peak is slightly shifted towards fuel-rich side (at lower value of $z$). Surprisingly formaldehyde concentration profile predicted using this reduced scheme agree with the results of the detailed model.

On the other hand, 1-D modeling results obtained with the scheme provided by Khare et al. [17] give more reasonable prediction of temperature in flame, OH and $O_2$ concentration profile, both very close to simulation with Burke et al. [15] scheme. However, over-prediction of a formaldehyde mole fraction (by the factor of 3) indicates some discrepancy of the given model reduction concerning minor species concentrations in flame. Although the brief comparison of DME oxidation schemes reported here is far from being complete and focuses mainly on HTC regime, it provides a clue for the preference of Khare et al. [17] scheme for 3-D modeling tasks.

Velocity and temperature profiles obtained from numerical simulations in the counter-flow are depicted in the Figure 4 and the Figure 5 respectively.

Figure 4: Contour plot of velocity from 3-D numerical simulations for the burner apparatus with 30° (A) and with 60° (B) tapers mounted on the bottom inlet nozzle

Figure 5: Contour plot of temperature from 3-D numerical simulations for the burner apparatus with 30° (A) and with 60° (B) tapers mounted on the bottom inlet nozzle
Relatively complex interactions of DME/oxygen mixture, co-flow shielding and counter-flowing heated nitrogen with strong inhomogeneity of velocity and temperature field in radial and axial directions can be seen for the case of 30° tapers. These effects are obviously less pronounced for the second case (60° tapers).

For both cases presented here, reaction zone is formed nearby the respective stagnation point. Presence of elevated concentrations of formaldehyde (CH$_3$O) and hydrogen peroxide (H$_2$O$_2$) being unambiguous product of LTC, i.e. marker of cool flame chemistry, is demonstrated in the Figure 6 and the Figure 7 respectively. Although the shape of reaction zone is not ideally flat spatially-distributed combustion diagnostics seems to be well applicable for determination of major and minor species profiles using line-of-the-sight optical methods. Based on these results we can infer that cool flame stabilization is achievable in the given experimental setup.

![Figure 6](image6.png)  
**Figure 6:** Contour plot of formaldehyde mole fraction X(CH$_2$O) obtained from 3-D numerical simulations for the burner apparatus with 30° (A) and with 60° (B) tapers mounted on the bottom inlet nozzle.

![Figure 7](image7.png)  
**Figure 7:** Contour plot of hydrogen peroxide mole fraction X(H$_2$O$_2$) obtained from 3-D numerical simulations for the burner apparatus with 30° (A) and with 60° (B) tapers mounted on the bottom inlet nozzle.
5 Conclusion

Interactions of fluid flow with detailed chemistry were investigated for the specific case of laminar counter-flow flame (double jet problem) by the means of 3-D numerical simulations. Relevant prediction of laminar counter-flow flame structure (i.e. temperature and species concentration profiles) was accomplished in complex burner geometry. Estimation of experimental conditions suitable for stabilization of a DME/oxygen cool flame in our counter-flow burner setup has been obtained in this way. Results concerning the proposed modifications of burner apparatus will be taken into account for development of optical/probe diagnostics for quantitative measurement of temperature profiles and species concentrations in laminar flames. A combined (modeling and experimental) methodology is further suitable for studying effects of dilution and chemical inhibition [19] (i.e. extinguishing processes) in the context of fire safety science.

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