MEASUREMENTS OF THE REACTIVITY OF PREMIXED, STAGNATION, METHANE-AIR FLAMES AT GAS TURBINE RELEVANT PressURES

Philippe Versailles
ASME Member
McGill University
Montréal, Canada

Antoine Durocher
ASME Student Member
McGill University
Montréal, Canada

Gilles Bourque
ASME Fellow
Combustion Key Expert
Siemens Canada Limited
Adjunct Professor
McGill University
Montréal, Canada

Jeffrey M. Bergthorson∗
ASME Member
Associate Professor
McGill University
Montréal, Canada

ABSTRACT
The adiabatic, unstrained, laminar flame speed, $S_L$, is a fundamental combustion property, and a premier target for the development and validation of thermochemical mechanisms. It is one of the leading parameters determining the turbulent flame speed, the flame position in burners and combustors, and the occurrence of transient processes, such as flashback and blowout. At pressures relevant to gas turbine engines, $S_L$ is generally extracted from the continuous expansion of a spherical reaction front in a combustion bomb. However, independent measurements obtained in different types of apparatuses are required to fully constrain thermochemical mechanisms. Here, a jet-wall, stagnation burner designed for operation at gas turbine relevant conditions is presented, and used to assess the reactivity of premixed, lean-to-rich, methane-air flames at pressures up to 16 atm. One-dimensional (1D) profiles of axial velocity are obtained on the centreline axis of the jet-wall burner using Particle Tracking Velocimetry, and compared to quasi-1D flame simulations performed with a selection of thermochemical mechanisms available in the literature. Significant discrepancies are observed between the numerical and experimental data, and among the predictions of the mechanisms. This motivates further chemical modeling efforts, and implies that designers in industry must carefully select the mechanisms employed for the development of gas turbine combustors.

INTRODUCTION
The adiabatic, unstrained, laminar flame speed, $S_L$, is one of the most fundamental properties in combustion science. Classical flame theory demonstrated that it is directly proportional to the square root of the overall rate of the combusting reaction [1, 2]. This makes $S_L$ a premier target for the development, validation, and optimization of thermochemical models utilized for the design of modern engines. Furthermore, it is the determining factor for transient events, such as flashback and blowout, in laboratory burners [3, 4], and it is commonly used to develop correlations describing their occurrence in more realis-
tic combustor geometries [5, 6]. The laminar flame speed is also employed as a scaling parameter in turbulent combustion, and is particularly important in the flamelet regime where the wrinkled flames retain, locally, their laminar structure [2, 7]. Finally, through its influence on the residence time within a fixed geometry, the flame speed was shown to have a direct impact on the formation of pollutants, such as nitrogen oxides [8–10].

Many laminar flame speed measurements at ambient conditions were reported over the last century [11–13]. They were performed in numerous types of apparatuses, such as Bunsen [14], stagnation [14–16], and porous plug / perforated plate [17, 18] burners, balloons [19], large enclosures [20] and bombs [21]. Improvements to the experimental methods, namely by accounting for aerodynamic stretch effects, allowed the variability originally observed among the data collected in independent facilities to be reconciled [11–13]. Over time, a large dataset of $S_L$ values was assembled for various types of inert, dilution levels, preheat temperatures, and fuels [12, 13, 22–25].

The ensemble of experimental data is not as broad at high pressures relevant to gas turbine engines. Most experiments were performed within combustion bombs in which the transient expansion of a spherical flame is tracked, generally by Schlieren photography, to yield the flame speed [12]. Single-chamber constant-volume, and dual-chamber quasi-isobaric bombs were used to study the propagation of premixed flames for a variety of fuels, preheat temperatures, and pressures beyond 50 bars [21, 26–30]. However, a wide set of accurate, independent measurements from different types of apparatuses is necessary to properly constrain thermochemical models used for engine design [31, 32]. Furthermore, potential discrepancies observed among the values obtained in different configurations can result in the discovery of unsuspected phenomena, as taught by the development of the aerodynamic stretch corrections [14].

Only a few attempts were made to investigate the reactivity of steady, burner-stabilized, premixed flames at high pressures; the increase in the Reynolds number that favors the transition to the turbulent flow regime, and the appearance of flame instabilities, make the stabilization of disturbance-free, laminar flames in burners very difficult [12, 29, 33]. Bunsen burners were used to study hydrogen-air [33] and $\text{H}_2/\text{CO}/\text{CO}_2/\text{O}_2/\text{He}$ [34] flames at pressures up to 5 and 15 atm, respectively. Also, the burning velocities of jet-wall, stagnation, syngas-air flames [35] and counterflow, stagnation, methane-air flames [29, 36, 37] were measured at pressures ranging from 1 to 5 atm, and 0.25 to 7 atm, respectively. Even if these studies provided important data for the understanding of flame propagation, and validation of thermochemical models, it appears that the dataset of experimental values of $S_L$ in burners at supra-atmospheric conditions is sparse, and generally limited to relatively low pressures [12].

In this context, the main objectives of the current paper are: 1) to complement the existing measurements with an independent set of flame reactivity data for lean-to-rich methane-air flames stabilized in a jet-wall, stagnation burner at pressures up to 16 atm; and 2) to test the accuracy of the thermochemical models used in industry to design gas turbine combustors. First, a complete description of the newly developed high-pressure, jet-wall, stagnation flame facility is provided. The Particle Tracking Velocimetry (PTV) technique utilized to measure the axial velocity profiles, and the quasi-one-dimensional modeling of stagnation flames are also discussed. Then, the predictions of seven thermochemical models are compared to the experimental data, and an uncertainty analysis is presented.

**METHODOLOGY**

The experiments reported herein were performed in a newly commissioned facility made of an optimized, jet-wall, stagnation burner installed in a high-pressure vessel. The rig is designed to allow continuous operation at the full-load pressure of modern aero-derivative gas turbine engines. In this section, the facility, the laser-based Particle Tracking Velocimetry technique, and the quasi-one-dimensional modeling of stagnation flames are presented.

**High-pressure, stagnation flame burner**

The jet-wall, stagnation burner is depicted in Fig. 1. A premixed jet of fuel and air flows through a converging nozzle with a throat diameter $D = 10.2$ mm (0.4 in) and impinges on a water-cooled stagnation surface placed $L \approx 9$ mm downstream of the nozzle assembly. In this configuration, the flame stabilizes at the location where its propagation speed balances the velocity of the decelerating flow. A co-flowing, annular stream of inert nitrogen gas surrounds the inner combustible jet to insulate the flame from the surroundings and improve its stability [38]. To prevent condensation and chemical reactions at the surface, the plate is maintained at a temperature between $420$ and $525$ K [39]. The plate temperature, and the heat loss it induces, have a negligible impact on the propagation speed of flames stabilized sufficiently upstream of the stagnation surface [39]. The axial position of the flames is carefully adjusted in the current experiments to ensure that their reactivity is evaluated at nearly adiabatic conditions and, therefore, solely dependent on the properties of the combustible mixture.

Type-K thermocouples, connected to a 24-bit isothermal data acquisition card (National Instruments NI 9214), are inserted in the feed lines and embedded 0.76 mm (0.030 in) into the plate to measure the temperatures of the reactants and stagnation surface, respectively. Digital mass flow controllers, calibrated using a DryCal ML-500 dry-piston calibrator equipped with ML-500-10 and ML-500-44 cells, meter the mass flow rate of the methane (Bronkhorst F-201CV-2K0-ABD-22-V), air (Bronkhorst F-201CV-10K-ABD-22-V), helium (Bronkhorst F-211CV-1K0-ABD-22-V), and nitrogen (Bronkhorst F-211AV-
50K-ABD-22-V) streams. To ensure homogeneity of the reactant mixture, it travels through a 38.1 mm (1.5 in) inner diameter (I.D.), 0.66 m (26 in) long mixing tank before entering the vessel. A flow settling section filled with 1 mm diameter alumina beads is also located upstream of the nozzle assembly (not shown in Fig. 1) to laminarize and homogenize the combustible and inert flows.

The burner is made of stainless steel alloy 316, and its geometry is optimized to provide laminar flames free of flow-induced disturbances at gas turbine relevant pressures. The interior contour of the inner nozzle was designed using a CFD-validated, Thwaites method [40]. The passage between the inner and outer nozzles (inert stream), the exterior surface of the outer nozzle, and the shape of the water-cooled stagnation plate were iteratively adjusted through a sequence of high-pressure CFD computations performed with Ansys Fluent. Namely, the plate shape is based on a NACA 6-series airfoil blended to a flat 10.2 mm diameter surface, and the exterior contour of the outer nozzle approximates a streamline of the flow induced by a point source jet [38]. The entire assembly was Computer Numerical Control (CNC) machined to realize the complex surfaces, and to provide the thinnest lips at the exit of the nozzles in order to minimize the extent of the wakes, and their impact on the flame.

![Diagram of the burner and its components](image)

**FIGURE 1.** JET-WALL STAGNATION BURNER.

**FIGURE 2.** COMPUTER-AIDED DESIGN MODEL OF THE APPARATUS.

**High-pressure vessel**

The burner is installed in a high-pressure vessel (see Fig. 2) designed based on the *ASME Boiler and Pressure Vessel code* [41] and the *Guide for Glass and Plastic Window Design for Pressure Vessels* of the Brookhaven National Laboratory [42]. It is capable of continuous operation at the full-load pressure of modern aero-derivative gas turbine combustors. The 0.29 m I.D. (11.5 in), 0.86 m (34 in) long enclosure is made of duplex and super-duplex grades of stainless steel, and features two pairs of 14.3 mm (9/16 in) thick, 57 mm (2.25 in) diameter (clear aperture) sapphire glass windows for laser-based diagnostics. To prevent water vapour condensation on the interior surfaces of the vessel, namely the windows, it is continuously purged by a stream of nitrogen gas. The pressure in the enclosure is regulated by a digital pressure controller (Bronkhorst P-522C-M10A-AGD-22-K) driving a pneumatic valve (Badger RCV RC200). The diaphragm-based, piezo-resistive sensor is calibrated using a NIST traceable, differential, digital pressure gauge (Ashcroft, full-scale of 800 psi(g), 0.05% accuracy of full-scale), whose zero is adjusted to the ambient conditions measured by the Drycal ML-500 calibrator (1.8 mmHg accuracy). This yields an overall uncertainty on the pressure of \( \sim 0.03 \text{ atm} \).

**Particle Tracking Velocimetry**

The axial velocity profiles are measured through two-dimensional Particle Tracking Velocimetry [10, 15, 43, 44]. A minimal amount of refractory scattering alumina particles (1 µm
diameter) is seeded in the inlet flow and irradiated by a thin (~1 mm) laser sheet aligned with the centreline axis of the burner. Borosilicate (N-BK7) glass lenses are used to vertically stretch and horizontally compress the beam emitted by a diode pumped, dual cavity, high-repetition rate Nd:YLF laser (Litron LDY 303, λ = 527 nm) time-controlled by a Stanford Research System DG535 pulse generator (0.0025% accuracy on the repetition rate). The frequency of the laser pulses (0.6 to 4 kHz) is adjusted for each experimental condition to maximize the resolution of the measurements in the low velocity region immediately upstream of the flame. The light scattered by the particles is collected using a Sigma 70-300 mm F4-5.6 macro lens mounted on extension tubes for improved magnification, and focused on a 14-bit monochrome, CCD camera (Cooke PCO.2000, 2048 × 2048 pixels²). The lens is equipped with a band-pass filter (Thorlabs FBH520-40 centred at 520 nm with a bandwidth at FWHM of 40 nm) to reject most of the interfering flame chemiluminescence. Several laser irradiation events are accumulated on single images exposed for as much as 350 milliseconds, which results in streaks of dots analogous to streamlines (see Fig. 3). The location of each dot (zp,i, rp,i) is computed through a grey scale intensity centroid calculation, and the individual, axial particle velocities, up(zp,i, rp,i), are calculated using the second-order accurate, central finite difference scheme of equation (1), where f [Hz] is the laser repetition rate, and C [m/pixel] is the spatial calibration coefficient determined from the image of a dotted target (Thorlabs R2L2S3P3, 500 ± 1 μm grid spacing, 250 μm dot diameter). A few tens of dot streaks in the vicinity of the centreline axis are superimposed to yield the one-dimensional profiles of axial velocity for each test case.

\[ u_p(z_{p,i}, r_{p,i}) \approx \frac{z_{p,i+1} - z_{p,i-1}}{2} \cdot f \cdot C \]  

(1)

**FIGURE 3.** PTV IMAGE OBTAINED IN A COLD, NON-REACTING FLOW.

**Quasi-one-dimensional flame modeling**

The laminar flame speed, \( S_u \), is a fundamental combustion parameter that corresponds to the velocity at which an unstrained, adiabatic, laminar, one-dimensional flame propagates. While this idealized flame can be simulated numerically, and its propagation speed readily predicted, it is unrealizable in the laboratory. In stagnation burners, \( S_u \) is traditionally extracted by extrapolating several strained reference flame speed measurements (\( S_u \), defined as the minimum axial velocity immediately upstream of the flame) obtained at various levels of strain rate (\( \dot{K} \), which corresponds for stagnation flames to the maximum value of \( dv/dz \) upstream of the reaction zone) to zero-stretch conditions [22]. However, the dependence between \( S_u \) and \( \dot{K} \) is a priori unknown, and a relationship needs to be hypothesized, which can induce significant inaccuracies in the extrapolated value of \( S_u \) [12]. Instead, to achieve the highest level of accuracy in the validation of the thermochemical models, the direct comparative approach is employed in which flame simulations exactly reproducing the experiments are benchmarked against the measured data [16, 45].

The simulations are performed with the quasi-one-dimensional (1D) stagnation flame model of Kee et al. [46] included in Cantera 2.3 [47]. This steady-state model assumes that the temperature, axial flow velocity, density, and species mole fractions are functions of the axial position, \( z \), only. Considering the axial symmetry of the jet-wall burner, the stream function \( \Psi(z,r) = \frac{1}{2} \cdot \rho(z) \cdot u(z) \cdot r^2 \) is assumed, which allows the three-dimensional Navier-Stokes, continuity, and energy and species conservation equations to be simplified to a quasi-1D formulation. The flame model takes as boundary conditions \( u_{inlet} \), \( (v/r)|_{inlet} \approx -1/2 \cdot du/dz|_{inlet} \), \( T_{inlet} \), and \( Y_i|_{inlet} \) at the inlet, and \( T_{wall} \), \( u_{wall} = 0 \), \( du/dz|_{wall} = 0 \), and \( [pY_i(u + V_i)|_{wall} = 0 \) at the stagnation surface. Good agreement is observed between simulations and experiments when the thermochemical model employed is accurate, the velocity boundary conditions (BC) are obtained from a parabolic fit to the velocity data upstream of the flame, and the motion of the PTV tracer particles is modeled to account for the thermophoretic force, inertia, Stokes drag, and gravity [16, 48, 49]. Namely, the quasi-one-dimensional flame model accurately predicts the axial profile of temperature, as well as the heat loss to the surface [8, 50]; the fields of axial and radial velocities, the boundary layer profile close to the wall, and the effects of flame stretch [15, 16]; and species concentration profiles [8, 10].

Table 1, in Appendix A, reports the boundary conditions determined experimentally. The inlet velocities and gradients are calculated 1 mm upstream of the flame front, in the cold-flow region where particle lag due to thermophoresis and high-curvature of the flow field is negligible. The values of \( u_{inlet} \) are obtained from parabolas least-squares fit to the experimental velocities, and the gradients from linear regressions to the experimental profiles of \( du_p/dz \) [10, 44]. The simulations are solved on meshes
refined to achieve gradient and curvature parameters of 0.05 and 0.075, respectively, and for relative and absolute tolerance levels of $10^{-3}$ and $10^{-9}$, respectively. Radiative heat losses and the mixture-averaged formulation of the diffusion coefficients are included in the simulations, while thermal (Soret) diffusion is neglected.

It is well-known that the refractory particles seeded for the purpose of velocimetry are plagued by a significant lag due to the combined effects of the thermophoretic force and inertia in high-gradient, high-curvature, chemically reactive flows [49,51,52]. It is an intricate task to remove these effects from the experimental particle velocities, and assumptions need to be made with regard to the temperature and species profiles, which are \textit{a priori} not known. This can introduce significant inaccuracies in the corrected velocity data. Instead, the particle velocities are predicted based on the flame simulations, which provide the required temperature and species profiles, by applying the model presented in [38,49]. Essentially, it applies Newton’s Second Law to a virtual refractory particle, and recovers its trajectory, $z_p(t)$, through temporal integration. To account for the fixed frequency of the laser, the finite difference scheme of equation (1) is applied to the numerical trajectory, which yields modeled particle velocities that can be directly compared to the experiments.

The velocity measurements reported in this study are used to benchmark the predictions of a selection of seven thermochemical models. GRI-Mech 3.0 (GRI) [53] was designed to simulate the combustion of natural gas, and is widely used in industry and academia. It includes 53 species and 325 reactions. It was globally optimized against a comprehensive set of experimental data, namely laminar flame speed measurements in counterflow burners and combustion bombs at pressures up to $\sim$ 20 atm.

Another model is the San Diego mechanism (SD) [54] that includes $C_1$-$C_4$ hydrocarbon and $C_1$-$C_2$ alcohol chemistry. The 2016 version considered in this study features 70 species, 321 reactions, and the $NO_x$ chemistry. This mechanism is optimized for pressures <100 atm and temperatures >1000 K, and differs from the other models by its design philosophy that aims for the minimal number of reactions and species to predict the combustion phenomena of interest.

The recently published model of the Combustion Science & Engineering, Inc. (CSE) firm [55] is also investigated. It includes 136 species and 966 reactions, and was designed to simulate the oxidation of $C_1$ to $C_4$ alkane fuels at low and high temperatures, as well as vitiated combustion. Its predictions were compared to burning speed measurements for pure and $CO_2$-diluted propane-air flames stabilized in Bunsen [55], counterflow [56], and jet-wall [57] burners at ambient pressure.

The largest of the mechanisms considered in this study was assembled at the National University of Ireland, Galway (NUIG). Its base chemistry derives from the model published in [58], which was validated against a comprehensive set of experimental flame speed data collected in burners and bombs, for various fuels and mixtures, at room and elevated pressures. It also comprises the nitrogen chemistry discussed and validated in [59]. The complete model contains 493 species and 2716 reactions. However, the reduced version for high temperatures, including 236 species and 1847 reactions, is used here.

An alternate mechanism is GDF-Kin 3.0 (GDF) [60], which was developed to model the combustion of natural gas. The $NO_x$ chemistry was removed for the current set of simulations: the so obtained $CH/CO$ chemistry has 100 species and 697 reactions. GDF-Kin 3.0 builds on GDF-Kin 2.0 [61], which was benchmarked against burning velocity data for $CH_4$-air, $C_2H_6$-air, and $C_3H_6$-air atmospheric flames.

The Konnov mechanism release 0.6 [62] is also compared to the current experimental data. The model uses 129 species and 1231 reactions to model the combustion of short-chain hydrocarbon fuels and $NO_x$ formation. It is the result of several iteratively improved mechanisms, which were validated against a broad range of experimental data, namely laminar burning velocities at pressures up to 10 atm.

The last model included in the validation is the high-temperature mechanism for $C_1$ to $C_3$ hydrocarbon fuels (version 1412), with $NO_x$ chemistry, prepared by the CRECK Modeling Group (CRECK) at Politecnico di Milano [63]. It features 115 species interacting through 2141 reactions, and was validated against a comprehensive set of laminar flame speeds obtained in jet-wall and counterflow burners, and combustion bombs, at pressures ranging from 0.5 to 60 atm [22].

**RESULTS AND DISCUSSION**

**Axial velocity measurements**

The experimental particle velocity profiles are shown in Fig. 4 for pressures of 2, 4, 8 and 16 atm, and equivalence ratios of 0.7, 0.8, 1.0 and 1.3. The figure is organized such that plots in the same row share the same equivalence ratio (different pressures), and plots in the same column feature the same pressure (different values of $\phi$). The combustible stream is flowing from right to left, the stagnation surface coincides with $z = 0$ mm, and the outlet of the inner nozzle is located at $z \approx 9$ mm. Higher pressures favor the appearance of flame instabilities. For the current experiments, the flames at $\phi = 0.8$, $P = 8$ atm (Fig. 4 (g)); $\phi = 1.3$, $P = 8$ atm (Fig. 4 (m)); $\phi = 0.8$, $P = 16$ atm (Fig. 4 (h)); and $\phi = 1.3$, $P = 16$ atm (Fig. 4 (n)) are diluted with 10% of inert helium gas per volume (i.e., $X_{He} = 0.1$ in the reactant stream) to damp these instabilities. It was impossible to stabilize the stoichiometric flames at 8 and 16 atm with this strategy and, therefore, no experimental data are provided for these conditions.

For all cases, the flow exiting the nozzle first decelerates, then rapidly accelerates through the flame front due to thermal expansion, and finally stagnates on the water-cooled surface. It must be noted that the reference flame speed, $S_u$, is commonly
FIGURE 4. PROFILES OF AXIAL PARTICLE VELOCITY. $P = 2$ ATM (FIRST COLUMN), $P = 4$ ATM (SECOND COLUMN), $P = 8$ ATM (THIRD COLUMN), AND $P = 16$ ATM (FOURTH COLUMN). $\phi = 0.7$ (FIRST ROW), $\phi = 0.8$ (SECOND ROW), $\phi = 1.0$ (THIRD ROW), AND $\phi = 1.3$ (FOURTH ROW).
based on the fluid velocity. However, the correction for the particle inertia, thermophoretic force, and finite frequency of the laser has a minimal impact upstream of the flame, such that reference flame speeds estimated from particle velocities are accurate. For pressures of 2 and 4 atm, it is observed, as expected, that $S_u$ is maximized at an equivalence ratio of unity, and decreases for richer and leaner mixtures. Considering the non-diluted $\phi = 0.7$ flames, it is noted that the reference flame speed decreases with pressure; a least-squares adjustment yields $S_u \propto P^{-0.71}$.

For all test cases, the experiments were reproduced numerically with Cantera 2.3 using the thermochemical models discussed previously, and taking as inputs the boundary conditions presented in Table 1. Note that only the NUIG, SD, CSE, and CRECK mechanisms include helium and, consequently, only these models are considered for the diluted flames. At all conditions, the models properly reproduce the qualitative behavior of the stagnation flame, i.e., an initial deceleration, followed by a rapid acceleration through the flame front, and finally a reduction of the axial velocity as the flow stagnates on the surface. For all mixtures and pressures, the GDF model over-predicts the reference flame speed; the flame stabilizes upstream (to the right) of the experimental flame front such that the overestimated value of $S_u$ balances with the incoming flow velocity. All other models are fairly consistent for $\phi \leq 1.0$ and $P \leq 4$ atm. For higher pressures, discrepancies among the models are noticed. The NUIG mechanism is the most accurate in terms of flame location and speed for $P \geq 8$ atm, while the CRECK model performs well for lean flames, but overestimates the reactivity of rich flames. Finally, for all pressures, there is a wide variability in the predictions of the models for $\phi = 1.3$.

For a few of these flames, e.g., at $\phi = 0.7$ and $P = 8$ atm, it is noted that, even though the predicted flame location and $S_u$ are relatively well captured by at least one of the models, the numerical and experimental velocity profiles do not agree in the post-flame region. The exact cause of this discrepancy has yet to be clearly identified, but ongoing work points toward second order, two-dimensional effects that are not captured by the quasi-one-dimensional hydrodynamic model.

**Uncertainty analysis**

The validation and optimization of thermochemical models require data of sufficiently high accuracy [31,32]: the uncertainty in the experimental values must be much smaller than the error in the flame reactivity predictions induced by the uncertain Arrhenius rate coefficients and inaccuracies in the structure of the models. The reference flame speed, $S_u$, a surrogate measure of the overall flame reactivity, is used as the metric for the current uncertainty analysis. The agreement between the simulations and the experiments is evaluated based on the ratio of the numerical and experimental values of $S_u$, which is calculated for all models and operating conditions (see Figs. 5 to 8). Exact agreement of the numerical predictions with the experimental data yields a nominal value of $S_{u,exp}/S_{u,exp} = 1$ (black, dashed line on the plots). For a few test cases, there are thermochemical models that over-predict the chemical reactivity to such an extent that the flame front travels all the way to the inlet of the computational domain (e.g., the rich, $P = 2$ atm flame computed with GDF). In this situation, a decelerating flow region is not observed upstream of the flame and, as a consequence, $S_u$ cannot be calculated, which explains why there are some data points missing in Figs. 5 to 8.

![Graph](image.png)

**FIGURE 5.** RATIO OF NUMERICAL TO EXPERIMENTAL VALUES OF $S_u$ FOR 2 ATM FLAMES. $S_{u,exp}/S_{u,exp} = 1$, SHOWN BY THE DASHED LINE, INDICATES EXACT AGREEMENT OF THE PREDICTIONS WITH THE EXPERIMENTAL DATA. THE SHADED GREY BAND PRESENTS THE ERROR RESULTING FROM THE UNCERTAINTIES IN THE BOUNDARY CONDITIONS, AND PTV EVALUATION OF $S_u$.

There are two main sources of uncertainty in the current experiments: 1) the error in the PTV measurements, $\delta_{S_u,exp, PTV}$, and 2) the uncertainty in the boundary conditions impacting the flame simulations, $\delta_{S_u, num, BC}$. The former is mainly caused by the uncertainty in the calibration coefficient ($C$), the laser repetition rate ($f$), the finite difference approximation of equation (1), and the scatter in the experimental data [44]. The total uncertainty on $S_{u,exp}$ is provided for each test case in Table 1 of Appendix A.

The error on the predicted reference flame speeds induced by the boundary conditions, $\delta_{S_u, num, BC}$, is obtained by propagating their uncertainty through the flame simulations. The logarithmic sensitivity of $S_{u, num}$ to the value of each BC, L.S.($x_j$), is ob-
\[ P = 4 \text{ atm} \]

\[ P = 8 \text{ atm} \]

\[ P = 16 \text{ atm} \]

\[ \frac{S_{u,\text{num}}}{S_{u,\text{exp}}} \]

\[ \phi \]

\[ (2) \]

\[ \delta S_{u,\text{num},\text{BC}} = \sqrt{\sum_j \left[ L \cdot S \left( x_j \right) \cdot \delta x_j \right]^2} \]

\[ \delta S_{u,\text{num}}/S_{u,\text{exp}} = 1 = \sqrt{\delta S_{u,\text{num},\text{BC}}^2 + \delta S_{u,\text{exp},\text{PTV}}^2} \]

\[ (3) \]

\[ \delta \]

\[ \sum \]

\[ \text{L.S.} \]

\[ x_j \]

\[ \delta x_j \]

\[ \text{BC} \]

\[ \text{PTV} \]

\[ \phi \]

\[ S_{u,\text{num}} \]

\[ S_{u,\text{exp}} \]

\[ \text{CONCLUSION} \]

The laminar flame speed is one of the most fundamental parameters in combustion. At high pressures relevant to gas turbine engines, most measurements were performed in combustion bombs. The current study extends the dataset of flame reactivity data by providing burning velocity measurements for
lean-to-rich, premixed, stagnation, methane-air flames at pressures up to 16 atm. The experiments were performed with a jet-wall burner optimized for operation at high pressures. Reference flame speeds predicted by seven thermochemical models were compared to the experiments. It was observed that while many mechanisms are fairly consistent and accurate for lean and stoichiometric flames at low pressures (2 and 4 atm), there are significant disagreements among the thermochemical models and against the experimental data at high pressures (8 and 16 atm), even if most of them were previously validated against reactivity data. This requires further work on chemical modeling, as well as added rigor in the selection of the experimental data used for the validation, and implies that professionals in industry must cautiously select the model they use for the design of combustors. Namely, they should make sure that it was thoroughly validated for their particular operating conditions, or verify its proper performance against the reference flame speed values provided in Appendix A.

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ACKNOWLEDGMENT

The authors gratefully acknowledge the support of BioFuelNet Canada, the Natural Sciences and Engineering Research Council of Canada (NSERC), the Fonds de recherche du Québec - Nature et technologies (FRQNT), and Siemens Canada Limited.

NOMENCLATURE

Thermochemical models
CRECK Politecnico di Milano [63]
CSE Combustion Science & Engineering, Inc. [55]
GDF Centre national de la recherche scientifique [60, 61]
GRI GRI-Mech 3.0 [53]
KON Lund University [62]
NUIG National University of Ireland, Galway [58, 59]
SD University of California, San Diego [54]

Symbols

\[ \begin{align*}
C & : \text{spatial calibration coefficient} \quad \text{m/pix} \\
D & : \text{throat diameter of the inner nozzle} \quad \text{m} \\
f & : \text{laser repetition rate} \quad \text{Hz} \\
l & : \text{length of the computational domain} \quad \text{m} \\
L & : \text{nozzle-to-plate separation distance} \quad \text{m} \\
L.S. & : \text{logarithmic sensitivity} \\
P & : \text{pressure} \quad \text{atm} \\
r & : \text{radial position} \quad \text{m} \\
r_{p,i} & : \text{particle radial position} \quad \text{pix} \\
S_L & : \text{unstrained, adiabatic, laminar flame speed} \quad \text{m/s} \\
S_u & : \text{strained reference flame speed} \quad \text{m/s} \\
t & : \text{time} \quad \text{s} \\
T & : \text{temperature} \quad \text{K} \\
u & : \text{flow axial velocity} \quad \text{m/s} \\
u_p & : \text{particle axial velocity} \quad \text{m/s} \\
v & : \text{flow radial velocity} \quad \text{m/s} \\
V_i & : \text{diffusional velocity of species } i \quad \text{m/s} \\
\chi_j & : \text{value of boundary condition } j \\
X_i & : \text{mole fraction of species } i \\
Y_i & : \text{mass fraction of species } i \\
z & : \text{axial position} \quad \text{m} \\
z_{p,i} & : \text{particle axial position} \quad \text{pix} \\
\rho & : \text{density} \quad \text{kg/m}^3
\end{align*} \]

Subscripts

exp : experimental value of the variable
inlet : at the inlet of the computational domain
num : numerically predicted value of the variable
wall : at the stagnation surface

REFERENCES


Appendix A: Experimental boundary conditions

Table 1 presents the boundary conditions for the stagnation flame simulations, as well as the experimental strained reference flame speed for each test case. The experimental uncertainty for each parameter is shown within parentheses.

Appendix B: Sensitivity and uncertainty analyses of the reference flame speed to the experimental boundary conditions

The determination of the uncertainty in the predicted reference flame speed induced by the boundary conditions starts with a brute-force sensitivity analysis. For each flame, the values of the boundary conditions \( x_j \) reported in Table 1 are perturbed sequentially by 1% in the quasi-one-dimensional flame simulations performed with the SD mechanism. Then, the logarithmic sensitivity of the reference flame speed to the individual boundary conditions is calculated as:

\[
\text{L.S.}(x_j) = \frac{\partial \ln S_u}{\partial \ln x_j} = \frac{\partial S_u}{\partial x_j} \cdot \frac{x_j}{S_u} \approx \frac{\Delta S_u}{\Delta x_j} \cdot \frac{x_{j,0}}{S_{u,0}},
\]

where \( x_{j,0} \) and \( S_{u,0} \) are the nominal values of the boundary conditions and reference flame speed, respectively, \( \Delta S_u \) is the change in \( S_u \), and \( \Delta x_j \) is the perturbation (\( \Delta x_j = 1.01 \cdot x_{j,0} - x_{j,0} \)).

Figures 9 (a) to 12 (a) present the results of the sensitivity analysis for the flames at 2, 4, 8 and 16 atm. On the figures, the bands are colored according to the equivalence ratio following a white (\( \phi = 0.7 \)) to black (\( \phi = 1.3 \)) colormap. The boundary condition having the largest influence on \( S_u \), i.e., the largest absolute value of L.S., is the equivalence ratio. As expected, the L.S. is positive for lean flames, i.e., increasing the equivalence ratio leads to a rise in the flame speed, and negative for rich flames (raising \( \phi \) for rich flames decreases \( S_u \)). It is followed by the temperature of the reactants, which tends to increase the reactivity of the flames, and the operating pressure. The other parameters have a more limited impact on the reference flame speed. It is worth to notice that the sensitivity of \( S_u \) to the plate temperature is low for most of the flames. This indicates that, as intended, the flames are stabilized sufficiently upstream of the stagnation surface for its temperature and, therefore, the convective heat loss, to have only a minimal effect on their reactivity.

The logarithmic sensitivity only describes how much a given parameter influences the reference flame speed. To quantify its contribution to the overall error on \( S_u \), its relative uncertainty (\( \delta x_j \)) must be multiplied by the corresponding value of L.S.\((x_j)\). Figures 9 (b) to 12 (b) show the product L.S.\((x_j) \cdot \delta x_j \). The values of \( \delta x_j \) are provided in Table 1. The main contributors to the uncertainty on \( S_u \) are, generally, \( \phi \) and \( T_{\text{inlet}} \). For the 2 atm flames, \( P \) is also inducing a non-negligible error on the reference flame speed and, at a few occasions, the velocity boundary conditions are also important. It must be noted, however, that significant efforts were made in preparing and performing the experiments to limit the uncertainty in the individual boundary...
TABLE 1. EXPERIMENTALLY DETERMINED BOUNDARY CONDITIONS FOR STAGNATION FLAME SIMULATIONS. THE ESTIMATED ABSOLUTE UNCERTAINTIES ARE SHOWN WITHIN PARENTHESES.

<table>
<thead>
<tr>
<th>$P$ [atm]</th>
<th>$\phi$</th>
<th>$l$ [mm]</th>
<th>$u_{inlet}$ [m/s]</th>
<th>$du_{inlet}/dz$ [1/s]</th>
<th>$T_{inlet}$ [°C]</th>
<th>$T_{wall}$ [°C]</th>
<th>$X_{He}$</th>
<th>$S_u$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 (0.03)</td>
<td>0.7 (0.005)</td>
<td>8.17 (0.05)</td>
<td>0.2029 (0.0008)</td>
<td>48.33 (4.91)</td>
<td>18 (2)</td>
<td>149 (5)</td>
<td>0 (0)</td>
<td>0.1544 (0.0013)</td>
</tr>
<tr>
<td>2 (0.03)</td>
<td>0.8 (0.006)</td>
<td>8.11 (0.05)</td>
<td>0.3205 (0.0010)</td>
<td>91.09 (1.96)</td>
<td>18 (2)</td>
<td>203 (5)</td>
<td>0 (0)</td>
<td>0.2218 (0.0027)</td>
</tr>
<tr>
<td>2 (0.03)</td>
<td>1.0 (0.007)</td>
<td>7.89 (0.05)</td>
<td>0.4805 (0.0014)</td>
<td>149.47 (2.31)</td>
<td>19 (2)</td>
<td>251 (5)</td>
<td>0 (0)</td>
<td>0.3145 (0.0069)</td>
</tr>
<tr>
<td>2 (0.03)</td>
<td>1.3 (0.009)</td>
<td>8.01 (0.05)</td>
<td>0.2812 (0.0008)</td>
<td>74.87 (2.25)</td>
<td>19 (2)</td>
<td>227 (5)</td>
<td>0 (0)</td>
<td>0.1994 (0.0019)</td>
</tr>
<tr>
<td>4 (0.03)</td>
<td>0.7 (0.005)</td>
<td>8.12 (0.05)</td>
<td>0.1288 (0.0004)</td>
<td>28.43 (2.31)</td>
<td>20 (2)</td>
<td>172 (5)</td>
<td>0 (0)</td>
<td>0.0980 (0.0009)</td>
</tr>
<tr>
<td>4 (0.03)</td>
<td>0.8 (0.006)</td>
<td>7.98 (0.05)</td>
<td>0.2281 (0.0008)</td>
<td>59.49 (2.81)</td>
<td>20 (2)</td>
<td>192 (5)</td>
<td>0 (0)</td>
<td>0.1533 (0.0029)</td>
</tr>
<tr>
<td>4 (0.03)</td>
<td>1.0 (0.007)</td>
<td>7.80 (0.05)</td>
<td>0.3806 (0.0012)</td>
<td>128.53 (3.79)</td>
<td>20 (2)</td>
<td>225 (5)</td>
<td>0 (0)</td>
<td>0.2448 (0.0041)</td>
</tr>
<tr>
<td>4 (0.03)</td>
<td>1.3 (0.009)</td>
<td>8.10 (0.05)</td>
<td>0.1938 (0.0006)</td>
<td>49.72 (2.40)</td>
<td>20 (2)</td>
<td>159 (5)</td>
<td>0 (0)</td>
<td>0.1390 (0.0028)</td>
</tr>
<tr>
<td>8 (0.03)</td>
<td>0.7 (0.005)</td>
<td>6.62 (0.05)</td>
<td>0.0754 (0.0002)</td>
<td>15.10 (0.94)</td>
<td>19 (2)</td>
<td>167 (5)</td>
<td>0 (0)</td>
<td>0.0588 (0.0012)</td>
</tr>
<tr>
<td>8 (0.03)</td>
<td>0.8 (0.006)</td>
<td>6.60 (0.05)</td>
<td>0.1181 (0.0006)</td>
<td>29.43 (1.24)</td>
<td>20 (2)</td>
<td>202 (5)</td>
<td>0.1 (0.0006)</td>
<td>0.0828 (0.0021)</td>
</tr>
<tr>
<td>8 (0.03)</td>
<td>1.3 (0.009)</td>
<td>5.73 (0.05)</td>
<td>0.0766 (0.0002)</td>
<td>15.20 (0.65)</td>
<td>20 (2)</td>
<td>188 (5)</td>
<td>0.1 (0.0006)</td>
<td>0.0579 (0.0007)</td>
</tr>
<tr>
<td>16 (0.03)</td>
<td>0.7 (0.005)</td>
<td>5.15 (0.05)</td>
<td>0.0473 (0.0001)</td>
<td>10.56 (0.75)</td>
<td>20 (2)</td>
<td>216 (5)</td>
<td>0 (0)</td>
<td>0.0357 (0.0006)</td>
</tr>
<tr>
<td>16 (0.03)</td>
<td>0.8 (0.006)</td>
<td>5.89 (0.05)</td>
<td>0.0623 (0.0002)</td>
<td>10.49 (0.56)</td>
<td>20 (2)</td>
<td>228 (5)</td>
<td>0.1 (0.0006)</td>
<td>0.0493 (0.0011)</td>
</tr>
<tr>
<td>16 (0.03)</td>
<td>1.3 (0.009)</td>
<td>4.94 (0.05)</td>
<td>0.0671 (0.0002)</td>
<td>16.76 (0.59)</td>
<td>20 (2)</td>
<td>235 (5)</td>
<td>0.1 (0.0006)</td>
<td>0.0464 (0.0010)</td>
</tr>
</tbody>
</table>

conditions ($\delta x_j$) so as to reduce their contribution ($L_i S_i (x_j) \cdot \delta x_j$) and the overall error in $S_{u, num}$. 

conditions ($\delta x_j$) so as to reduce their contribution ($L_i S_i (x_j) \cdot \delta x_j$) and the overall error in $S_{u, num}$. 

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FIGURE 10. (a) LOGARITHMIC SENSITIVITY OF $S_u$ TO THE VALUE OF THE BOUNDARY CONDITIONS ($x_j$), AND (b) CONTRIBUTION OF THE INDIVIDUAL BOUNDARY CONDITIONS TO THE OVERALL ERROR ON $S_u$ AT $P = 4$ atm. SAME LEGEND AS FIG. 9.

FIGURE 11. (a) LOGARITHMIC SENSITIVITY OF $S_u$ TO THE VALUE OF THE BOUNDARY CONDITIONS ($x_j$), AND (b) CONTRIBUTION OF THE INDIVIDUAL BOUNDARY CONDITIONS TO THE OVERALL ERROR ON $S_u$ AT $P = 8$ atm. SAME LEGEND AS FIG. 9.
FIGURE 12. (a) LOGARITHMIC SENSITIVITY OF $S_u$ TO THE VALUE OF THE BOUNDARY CONDITIONS ($x_j$), AND (b) CONTRIBUTION OF THE INDIVIDUAL BOUNDARY CONDITIONS TO THE OVERALL ERROR ON $S_u$ AT $P = 16$ ATM. SAME LEGEND AS FIG. 9.