Accurate determination of syngas flame speeds and validation of kinetic mechanisms

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Objectives

Coal-based Integrated Gasification Combined-Cycle (IGCC) systems offer an opportunity for utilizing an abundant and relatively cheap resource for power generation while still controlling air pollutant emissions, achieving high energy conversion efficiencies, and sequestering carbon. A successful design of reliable and efficient gas turbine engines operating on high hydrogen content syngas fuels strongly depends on knowledge of the combustion and radiation properties of syngas at actual gas turbine conditions and on the availability of reliable chemical kinetic and radiation models for numerical modeling. Unfortunately, very limited experimental data of syngas and hydrogen burning properties such as flame speeds and flammability limits at high pressures are currently available. The objectives of the present study are to characterize and model the radiation properties of combusting syngas, accurately measure syngas flame speeds at higher pressures, and develop reliable chemical kinetic models for syngas oxidation. In order to accomplish these objectives, several improvements to flame speed measurement using spherical flames were developed that significantly enhance the accuracy of the experimental data gathered in the present study.

Accomplishments to Date

A new fitted statistical narrow-band correlated-k (FSNB-CK) model was developed and validated for accurate radiation prediction in spherical geometry. The effects of spectral radiation absorption on the flame speed at normal and elevated pressures were experimentally and numerically investigated using the CO_2 diluted outwardly propagating CH_4-O_2-He flames. The results showed that radiation absorption with CO_2 addition increases the flame speed and extends the flammability limit. Contrary to conventional theory, increasing pressure augments the effect of radiation absorption. The present model was demonstrated to perform better the SNB gray gas model and optically thin model. Neither adiabatic nor optically thin radiation models can provide kinetic validation at high pressure and near limit conditions.

The accuracy of the spherical flame method for experimental flame speed determination was investigated and several improvements to the method were developed. For flame speed measurement using spherical flames in non-spherical chambers, the effect of non-uniform flow disturbances was found to have a significant effect on the determination of burning velocities. A *flow-corrected flame speed* was developed to account for the actual induced motions in the burned gas and it was shown to improve the accuracy of flame speed determination significantly. In spherical chambers, a similar effect is caused by compression-induced burned gas motions due to pressure rise during the combustion process. A *compression-corrected flame speed* developed in this study was demonstrated to give more reliable results. Additionally, transient effects caused by ignition were shown to alter the flame radius-time trajectories from the quasi-steady branch during early propagation of the flame—thus invalidating the use of the commonly employed quasi-steady theory to interpret the experimental results. It is suggested that only flame radii large enough that these transient effects have decayed are used for flame speed determination using quasi-steady theory.

Laminar flame speeds were measured experimentally using these improved methods for spherical flames for H_2/CO/CO_2/dilutent mixtures over equivalence ratios from 0.5 to 4.0, CO_2 dilution ratios from 0 to

25%, and pressures from 1 to 25 atm. The results for extrapolated burning velocity are compared to planar predictions by recent kinetic mechanisms for syngas combustion. The comparisons reveal large differences among the models and large differences between the experimental data and the model predictions under some conditions at high pressures, indicating that significant modifications of the existing mechanisms are necessary to extend them into the high pressure regime.

Future Work

The source of the high-pressure flame speed discrepancies is currently under investigation. Preparations for measuring high temperature, water-diluted flame speeds are underway. Production of a reduced mechanism from our detailed kinetic mechanism is planned.

Journal Papers Published

1. M.P. Burke, Z. Chen, Y. Ju, F.L. Dryer, "On the Determination of Laminar Flame Speed Using Outwardly Propagating Flames: Effect of Cylindrical Confinement", submitted for publication.
2. Z. Chen, M.P. Burke, Y. Ju, "On the Accurate Determination of Laminar Flame Speed from Expanding Spherical Flames: Effect of Initial Flame Transition", accepted for *Proceedings of the Combustion Institute* (2009).
3. Z. Chen, M.P. Burke, Y. Ju, "Effects of compression and stretch on the determination of laminar flame speed using propagating spherical flames", submitted for publication.
4. Z. Chen, Y. Ju, "Combined effects of curvature, radiation, and stretch on the extinction of premixed tubular flames", submitted for publication.
5. Z. Chen, X. Qin, B. Xu, Y. Ju, F. Liu, "Studies of radiation absorption on flame speed and flammability limit of CO2 diluted methane flames at elevated pressures", *Proceedings of the Combustion Institute* (2007) 31: 2693-2700.

Conference Presentations

1. M.P. Burke, Y. Ju, F.L. Dryer, "Effect of Flow Field Perturbations on Laminar Flame Speed Determination Using Spherical Flames", 46th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, USA, January 2008.
2. Z. Chen, M.P. Burke, Y. Ju, "Effects of Lewis Number on Spherical Flame Transition", 46th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, USA, January 2008.
3. Z. Chen, Y. Ju, "The stretch effect on the accurate determination of laminar flame speed using expanding flames in a spherical bomb", Eastern States Meeting of the Combustion Institute, Charlottesville, Virginia, USA, October 2007.
4. M.P. Burke, Y. Ju, F.L. Dryer, "Effect of Cylindrical Confinement on the Evolution of Outwardly Propagating Flames," Eastern States Meeting of the Combustion Institute, Charlottesville, Virginia, USA, October 2007.
5. Z. Chen, Y. Ju, "On the accurate determination of flame speeds at normal and elevated pressures by using a spherical bomb: the effect of compression and stretch", 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, USA, January 2007. No. 2006-0378.
6. Z. Chen, Y. Ju, "The effects of flow compression on the determination of flame speeds using propagating spherical flames at normal and elevated pressures", 5th US Combustion Meeting, San Diego, California, USA March 2007.
7. M.P. Burke, X. Qin, Y. Ju, F.L. Dryer, "Measurements of Hydrogen Syngas Flame Speeds at Elevated Pressures," 5th US Combustion Meeting, San Diego, California, USA, March 2007.
8. Z. Chen, Y. Ju, "On the accurate determination of flame speeds at normal and elevated pressures by using a spherical bomb: the effect of compression and stretch (detailed chemistry)", 6th Asian-Pacific Conference on Combustion (ASPACC07), Nagoya, Japan, May 2007.

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