Structure of premixed flames of H_2/CO mixtures at atmospheric pressure: experimental and numerical study

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Elaboration of a predictive and well validated kinetic mechanism for combustion of H_2/CO mixtures is the key to development of advanced technologies for effective burning of syngas in power generation systems. Moreover, understanding the combustion chemistry of H_2/CO mixtures is a prerequisite for a comprehensive description of the chemistry of hydrocarbons and development of predictive chemical kinetic models for combustion of transportation fuels. Despite extensive experimental efforts to examine combustion characteristics of syngas and therefore validate available chemical kinetic models for syngas combustion, there is a lack of experimental data on the concentrations of intermediates in flame conditions, in particular, at pressures close to atmospheric. In our recent work we succeeded in measurements of many intermediates, including O, OH, HO_2 radicals, in a stoichiometric premixed burner-stabilized H_2/CO/O_2/Ar flame at 5 atm [D. A. Knyazkov, T. A. Bolshova, A. M. Dmitriev, A. G. Shmakov, O. P. Korobeinichev, Combustion, Explosion, and Shock Waves, 2017, Vol. 53, No. 4, pp. 388–397]. However, working at the elevated pressure, we encountered difficulties to stabilize the H2/CO flame in the range of equivalence ratios, so the experimental data were reported only for the stoichiometric flame.

In this work we report new experimental data for chemical speciation in the atmospheric pressure burner-stabilized premixed flames diluted with Ar and fuelled with H_2/CO (1:1) mixture at equivalence ratios of 1 and 2. In atmospheric pressure conditions we were able to span a wide range of equivalence ratios and therefore to reveal the tendencies observed with the change in the unburnt mixture composition. The goal was to ascertain how the available models for syngas combustion reproduce these tendencies, particularly for labile flame intermediates. This will allow a formulation of guidance for further development of predicative kinetic schemes of syngas combustion.

Flame sampling molecular beam mass spectrometric setup with soft electron impact ionization was used in this work to examine laminar premixed flames of H_2/CO/O_2/Ar mixtures stabilized on a Botha-Spalding burner. Argon mole fraction in the mixtures was 0.75. The flames were sampled by a sonic quartz probe with 0.07 mm orifice diameter. Spatial variations above the burner of mole fractions of reactants (H_2,CO, O_2), major flame products (H_2O, CO_2) and intermediates (H, O, OH, HO_2, H_2O_2) were measured.

Recent detailed chemical kinetic mechanisms for syngas combustion available from literature were used to simulate the experimental profiles with the CHEMKIN package of codes. Kinetic analysis of the mechanisms allowed explaining the observed tendencies with the change of equivalence ratio.

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