

Flame Dynamics in Supercritical Condition

Research Component of PhD General Exam

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Abstract:

Combustion under high-pressure conditions holds the potential for improved thermodynamic efficiency, enhanced power generation, and reduced emission of some pollutants. It underlies the technology of internal combustion engines such as the automotive engine, the gas turbine, and the rocket engine, for which the operating pressure can reach as high as 100s atm. At such high-pressure conditions, the fluids can be locally or even globally at the supercritical state, and as such are subjected to considerable real-fluid effects. Recognizing that studies of high-pressure combustion frequently adopted ideal-gas approximations to describe the thermodynamics, transport and chemical kinetics components of the problem, it behoove us to assess the extent of accuracy embedded in such approximations. Most previous investigations on supercritical or transcritical combustion have focused on diffusion flames. Only limited studies, however, have been conducted on premixed flames at supercritical conditions. Therefore, this study aims to computationally simulate propagation of hydrogen and methane flames in supercritical conditions for the planar and spherical configurations, incorporating descriptions of supercritical thermodynamics, transport and chemical kinetics. It consists of four parts:

First, recognizing that most previous investigation involved hydrogen flames, methane flames were also included in the present study, as methane not only is the simplest hydrocarbon, it is also relevant for high-pressure applications including rocket propulsion and methane-hydrate utilization.

Second, the effects of various aspects of non-ideality for the laminar flame propagation were identified at progressively more complete levels of formulation. Specifically, for hydrogen/air flames, the laminar flame speeds at high pressures were found to increase due to the non-ideal equation of state (EoS), and is mainly due to the density modification of the initial mixture. On the other hand, including the thermodynamic properties of enthalpy and heat capacity reduces the flame speed because of the correspondingly reduced adiabatic flame temperature. Transport properties were found to have small effect because of the decoupled transport modification with the main reaction zone.

Third, a recently developed high-pressure methane oxidation mechanism was incorporated in the simulation, thereby provide a first effort in assessing the influence of high-pressure

chemistry on the flame response. It is noted that the importance of realistic description of chemistry is essential for such practical problem as flame stabilization and blow-off, and for such fundamental issue as the meaningful extraction of chemical kinetics from the experimental data of laminar flame speeds. For the methane/air flames, the use of recently reported high-pressure chemical kinetics considerably affects the laminar flame speed determined by using the low-pressure reaction schemes.

Fourth, the influence of aerodynamic stretch on supercritical flames was also investigated, the essential coupling between stretch and mixture non-equidiffusion, and how supercritical modification of the mixture diffusivities could affect the dynamic response of flames. For the spherical flame simulation, hydrogen/air flame at high pressures demonstrates that supercritical mixtures exhibit enhanced Lewis number, which leads to hindered/enhanced Lewis number effect for lean/rich hydrogen/air stretched flames.