Combustion kinetics: experiments, analysis, reduction and use in fundamental and applied numerical investigations

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The experimental and numerical work at LAV addresses different aspects of combustion kinetics. Primary reference fuels and synthetic fuels are investigated experimentally in an optically accessible rapid compression expansion machine (RCEM) under homogeneous conditions for a variety of initial charge temperatures, equivalence ratios and simulated exhaust gas recirculation. The experiments provide transient ignition delay and heat release rate data, while OH-chemiluminescence and spectrography measurements give insight into the combustion process. The data is used on one hand to tune simple predictive autoignition models capable of describing both the negative temperature coefficient behavior of the main ignition and the low temperature reaction ignition. On the other hand, they are employed for validation of detailed reaction mechanisms by comparison with homogeneous autoignition calculations [1].

Numerical investigations cover mechanism analysis, reduction and use of reaction mechanisms in the direct numerical simulation (DNS) of fundamental combustion phenomena, and in the large eddy and Reynolds-averaged Navier-Stokes (LES and RANS) of practical applications in internal combustion engines (ICEs) and other combustion setups. The analysis of detailed reaction mechanisms for gas phase [2] as well as surface chemistry [3] employs the tools provided by the Computational Singular Perturbation (CSP) method. Reduced descriptions have been constructed using existing and newly proposed methods based on the notion of slow invariant manifold (SIM). Iteratively refined approximations of the SIM have been constructed using the method of invariant grids [4] and the global relaxation redistribution method [5]. Recently, an easy to implement method based on the contribution of elementary reactions to the total entropy production was proposed for the construction of a significantly simpler skeletal mechanism for n-heptane [6], which was used to systematically study complex dynamics of a higher hydrocarbon fuel in perfectly stirred reactors using continuation and bifurcation analysis [2].

DNSs have mainly employed detailed reaction mechanisms of simple fuels like hydrogen or syngas to study laminar and turbulent non-premixed, premixed combustion and autoignition in jets in co- and cross-flows as well as in closed cylindrical geometries under HCCI conditions. Detailed or reduced mechanisms in multi-dimensional RANS/LES for ICEs and other setups are accounted for by Conditional Moment Closure (CMC) models implemented in commercial and open source solvers (e.g. [7], [8], [9]).

References

[1] D. Mitakos, C. Blomberg, A. Vandersickel, Y.M Wright, B. Schneider, K. Boulouchos, Ignition Delays of Different Homogeneous Fuel-air Mixtures in a Rapid Compression Expansion Machine and Comparison with a 3-Stage-ignition Model Parameterized on Shock Tube Data, *SAE Int. J. Engines* 6(4):1934-1952, 2013

[2] M. Kooshkbaghi, C.E. Frouzakis, E. Chiavazzo, K. Boulouchos, I.V. Karlin, *n*-heptane/air combustion in perfectly stirred reactors: Dynamics, bifurcations and dominant reactions at critical conditions, *Combust. Flame*, doi:10.1016/j.combustflame.2015.05.002

[3] A. Brambilla, C.E. Frouzakis, J. Mantzaras, A. Tomboulides, S. Kerkemeier, K. Boulouchos, Detailed transient numerical simulation of H2/air hetero-/homogeneous combustion in platinum-coated channels with conjugate heat transfer, *Combust. Flame*, 161(10), 2692-2707, 2014

[4] E. Chiavazzo, I.V. Karlin, C.E. Frouzakis, K. Boulouchos, Method of invariant grid for model reduction of hydrogen combustion, *Proc. Combust. Inst.*, 32(1), 519-526, 2009

[5] M. Kooshkbaghi, C.E. Frouzakis, E. Chiavazzo, K. Boulouchos, I.V. Karlin, The global relaxation redistribution method for reduction of combustion kinetics, J. *Chem. Phys.*, 141(4):044102, 2014

[6] M. Kooshkbaghi, C.E. Frouzakis, K. Boulouchos, I.V. Karlin, Entropy production analysis for mechanism reduction, *Combust. Flame*, 161(6), 1507-1515, 2014

[7] Y.M. Wright, G. De Paola, K. Boulouchos, E. Mastorakos, Simulations of spray autoignition and flame establishment with two-dimensional CMC, *Combust. Flame,* 143 (4), 402-419, 2005

[8] Y.M. Wright, O.N. Margari, K. Boulouchos, G. De Paola, E. Mastorakos, Experiments and simulations of n-heptane spray auto-ignition in a closed combustion chamber at diesel engine conditions, *Flow Turb. Combust.*, 84 (1), 49-78, 2010

[9] M. Bolla, T. Gudmundsson, Y.M. Wright, K. Boulouchos: Simulation of Diesel Sprays using the Conditional Moment Closure Model*, SAE Int. J. Engines* 6 (2), 1249-1261