

# A study of strained extinction for applications in natural gas combustion modeling

by

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## Technical Summary

Resistance to extinction by stretch is a key property of any flame, and recent work has shown that this property controls the overall structure of several important methane, the principal component of natural gas, based turbulent flames. This work gives an introduction to the parameter that quantifies resistance to extinction by stretch, Extinction Strain Rate (ESR), discussing how it is typically measured experimentally and calculated numerically. The primary limitations of ESR given its historical definition and computation methods are (1) it depends on the dimensions of the experimental apparatus used to measure it (2) it is often too computationally difficult to calculate using large kinetic models,  $\#species > 500$ , and (3) under elevated pressures relevant to gas turbines and internal combustion engines, 20-40 atm, it is difficult to measure. Work addressing in some manner these three issues is presented. Subsequent work then uses ESR as a validation parameter for producing a kinetic model.

To address the first issue, a method is proposed for translating experimental measurements for stretch-induced extinction into an unambiguous and apparatus-independent quantity ( $ESR_{\infty}$ ) by extrapolating to infinite opposing burner separation distance. The uniqueness of the flame at extinction is shown numerically and supported experimentally for twin premixed, single premixed, and diffusion flames at Lewis numbers greater than and less than one. A method for deriving  $ESR_{\infty}$  from finite-boundary experimental studies is proposed and demonstrated for methane and propane diffusion and premixed single flame data. The values agree within the range of differences typically observed between experimental measurements and simulation results for the traditional ESR definition.

To address issue two, Ember, a new open-source code for efficiently performing  $ESR_{\infty}$  calculations using large, detailed chemical kinetic models is presented. Ember outperforms other standard software, such as Chemkin, in computation time by leveraging rebalanced Strang operator splitting which does not suffer the steady-state inaccuracies of most splitting methods. Ember is then able to improve computational performance primarily through parallelization and use of quasi-steady-state kinetics integrations at each independent spatial discretization point. Ember is validated for computation of ESR and the benefits of its computation techniques are demonstrated.

With respect to the third issue, Ember is used to explore  $ESR_{\infty}$  pressure trends and kinetic model sensitivities in the current absence of experimental methods to probe the relevant parameter space. ESR shows opposing trends with pressure under lean and rich conditions for methane-air flames. Ultimately, ESR decreases at higher pressures for lean conditions ( $\phi = 0.7$ ) and increases with pressure for rich conditions ( $\phi = 1.3$ ). Under both conditions, the ESR trends are non-monotonic. ESR reaction sensitivities are observed to generally mirror those of laminar flame speed calculations. This suggests that there is limited added value in more efficient methods of ESR reaction sensitivity calculation since efficient adjoint methods already exist for laminar flame speed. Strong species transport parameter sensitivities are observed for the fuel, oxidizer, and bath gas, with the limiting reactant showing the strongest sensitivity. Current levels of uncertainty in species enthalpy suggest little impact of enthalpy errors on ESR predictions for the conditions studied.

Using the prior ESR improvements and analysis, an ESR validated kinetic model is produced. The model uses a validation data set that includes relevant ignition delay, laminar flame speed, and extinction strain rate data. The work builds off recent works by Hashemi and coworkers for high pressure oxidation of small hydrocarbons. Prediction of the selected validation data set is improved primarily through sensitivity analysis and comparison with kinetic rate constants from other works. Additionally, to support nitrogen chemistry predictions, the full nitrogen subset from the recent review by Glarborg and coworkers is appended to the core model produced. The Reaction Mechanism Generator (RMG) software has been recently used to generate the rich chemistry relevant for partial partial oxidation of methane up to one and two ring aromatics. This rich chemistry subset is added to produce the final kinetic model.

An important portion of the rich chemistry included within the produced kinetic model is the route from cyclopentadienyl radical recombination to naphthalene. Since this work seeks performance at elevated pressures of relevance to gas turbines and internal combustion engines, the pathway is re-computed here with explicit consideration of all relevant pressure dependent pathways on the  $C_{10}H_{10}$  and  $C_{10}H_9$  surfaces. Lumped, single step kinetics often used to describe the net reaction to naphthalene are observed to be insufficient. Specifically, the  $C_{10}H_{10}$  intermediate species is observed to live long enough undergo bimolecular reaction to enter the  $C_{10}H_9$  surface before proceeding on to naphthalene. Rate expressions for the full network are produced and included in the kinetic model generated.

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