Detailed Modeling of Flame-Wall-Interactions under the influence of phosphorous-containing Flame Retardants and development of a reduced kinetic model

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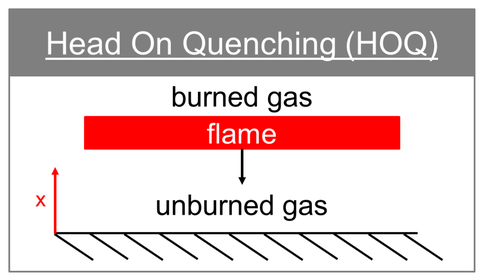
Motivation

- Critical role of flame retardants in fire safety engineering necessitates understanding of impact on combustion processes
- Numerical modeling helps to analyze the processes
- Complex reaction mechanisms and different time scales lead to high dimension and stiffness of partial differential equation system resulting in high CPU time ➡ Reduction of CPU time by using reduced kinetic models
- REDIMs are used to capture and to describe complete extinction process and influence of flame retardants

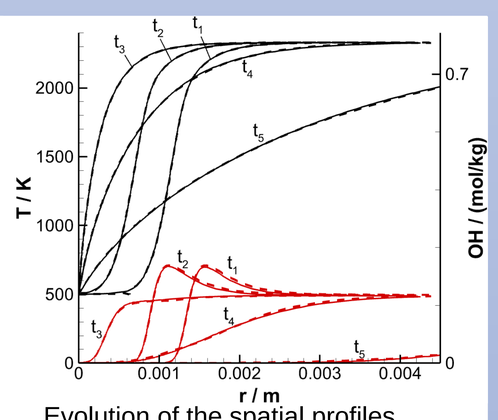
Model system and methodology

- Premixed stoichiometric Methane/Air/DMMP flame traveling towards a cold wall with T=500K
- Flame-Wall Interaction with Head-On-Quenching using Jayaweera Mechanism [1] for DMMP
- Reduction using Reaction-Diffusion Manifold (REDIM) method [2]
  - The inhibiting character of the flame retardant challenges the generation of the reduced kinetics due to the complexity of the chemical system
  - Assuming that only a few reactive and diffusive processes couple, the fast and very slow time scales can be decoupled and the slow scales are coupled to the transport processes. The states during combustion processes are constrained to a low dimensional manifold, which can be parameterized by a small number of variables, represented by the vector θ of generalized coordinates.
  - Evolution equation for REDIM : $\frac{\partial \psi}{\partial t} = (\boldsymbol{I} - \psi_\theta \psi_\theta^+)\left\{\boldsymbol{F} + \frac{1}{\rho}(\boldsymbol{D}\psi_\theta \chi)_\theta \chi\right\}$
  - Gradient estimate $\chi = \psi_\theta^+ \mathrm{grad}(\psi)$ of the physical variables and initial guess are obtained from detailed sample solutions
  - Manifold parametrized by 2 dimensions describing the heat loss towards the wall and the progress of chemical reaction
  - The stationary solution ($t \to \infty$) of the REDIM equation provides the REDIM; $\psi(\theta), \psi_\theta^+, \psi_\theta^+ \boldsymbol{F}$ & $\boldsymbol{D}\psi_\theta$ are tabulated at every grid point

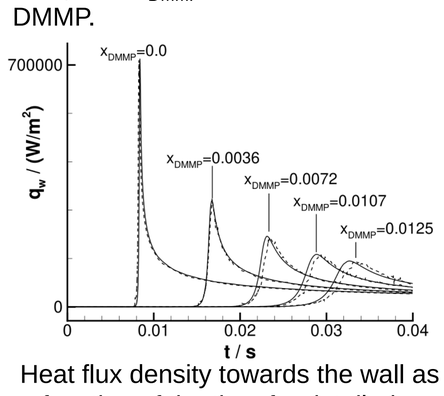


Results

- Comparison of detailed and reduced calculations
  - REDIM method can be used for flame wall interaction of phosphorous-containing flame retardants (good agreement of detailed and reduced kinetics)
  - REDIM captures the influence of added DMMP and correctly reproduces the system dynamics
- Comparison of maximum gradients of the temperature
  - Temperature is higher, width of flame front lower and flame speed larger for less DMMP
  - Temporal investigation of heat flux density to the wall allows a comparison between the flame velocities and the transferred heat

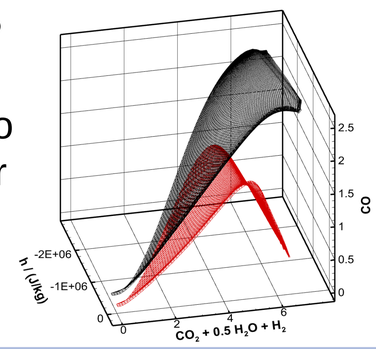


Evolution of the spatial profiles ($t_1<t_2<t_3<t_4<t_5$) of the temperature (black) and the specific mole numbers of OH (red). Detailed kinetics (solid lines) and reduced kinetics (dashed lines) with x_{DMMP} = 0.0018 of added DMMP.



Heat flux density towards the wall as a function of the time for detailed and reduced kinetics with different amounts of added DMMP.

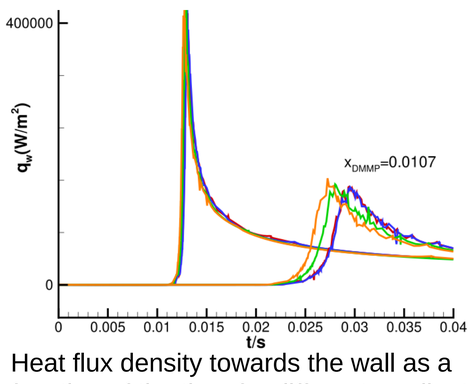
- The addition of DMMP leads to different assessed states due to the inhibiting character of phosphorous compounds



REDIMs of the stoichiometric flame without flame retardants (red) and with added DMMP (x_{DMMP} = 0.0125, black) in the state space. The species are given in mol/kg and the specific enthalpy h in J/kg.

Sensitivity analysis

- Investigation of the sensitivity of the reduced calculation on the gradient estimate
- Varying gradient estimate from detailed calculation by variable α from 0.5 to 2.0: $\mathrm{grad}\psi = \alpha \cdot \mathrm{grad}\psi_{det}$
- Overall good agreement for all α
- For increasing α:
  - Time of the maximum heat flux density occurs earlier (more significant at higher DMMP concentrations) due to higher flame speed
- Simulation is more sensitive with respect to the gradient estimate for higher amounts of DMMP



Heat flux density towards the wall as a function of the time for different gradient estimates $\mathrm{grad}\psi_{det}$ (red) and $\mathrm{grad}\psi$ with $\alpha = 0.5$ (blue), $\alpha = 1.5$ (green), $\alpha = 2.0$ (orange).

References

- [1] T. Jayaweera, C. Melius, W. Pitz, C. Westbrook, O. Korobeinichev, V. Shvartsberg, A. Shmakov, I. Rybitskaya, H. J. Curran, *Flame inhibition by phosphorus-containing compounds over a range of equivalence ratios*, Combust. Flame 140 (1-2) (2005) 103–115
- [2] V. Bykov, U. Maas, *The extension of the ILDM concept to reaction–diffusion manifolds*, Combust. Theor. Model. 11 (6) (2007) 839–862

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