Spherically Expanding Flame Simulations in Cantera Using a Lagrangian Formulation

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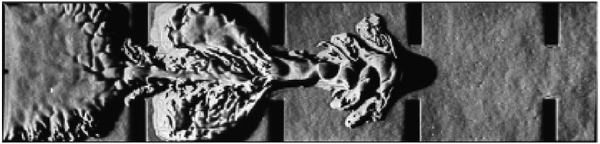
Introduction:

- Lean H_2-air mixtures with high stretch rates:
  - Develop cellular instability
  - $-$ve Markstein (Ma) number and $\uparrow$ burning rates
  - Contributes to flame acceleration (FA) and DDT
- Rich H_2-air mixtures with high stretch rates:
  - More stable
  - Delayed FA and DDT
- **Characterization of the response of the flame to stretch is of primary importance for risk assessments**



FA in 10% H_2-air [Matsukov et al. 1999]

Past investigations on influence of flame stretch:

- 1-D simulations of spherical H_2-air flames:
  - Effect of stretch on temperature and radical formation vs. unstretched flames [Aung et al., 1997]
    - $\uparrow$ flame speed for unstable lean H_2-air mixtures due to a “more nearly stoichiometric” mixture formed due to the preferential diffusion of H2
  - Stretched flames with He and Ar dilution [Kwon and Faeth, 2001]
  - Global parameter measurements independent of flame configuration, i.e. outward vs. inward [Sun et al., 1999]
  - Comparison of lean H_2-air mixtures to experimental data 30% discrepancy [Varea et al., 2015]
- **Such 1D codes not open-source or freely available**

Goals of this work:

1. Create open-source code to simulate 1-D unsteady spherically expanding flames
   - Based on old run-1DL code in Lagrangian coordinates [Rogg and Wang, 1995] (not publicly available)
2. Validation of flame speed and Ma to lean/rich H_2-air experiments (for $0.3 \leq \phi \leq 5,\ T_1 = 300\mathrm{K},\ p_1 = 101\mathrm{kPa}$)
3. Examine the flame dynamics of lean/rich hydrogen-air mixtures

Numerical Method:

$$\underbrace{\rho\frac{\partial Y_i}{\partial t}}_{\Delta \text{ mass (specie i)}} = \underbrace{\dot{\omega}_i}_{\text{production rate}} - \underbrace{\rho\frac{\partial(\rho r^2 u_{d,i} Y_i)}{\partial m}}_{\text{diffusion}} \quad (1)$$

$$\underbrace{\rho c_p \frac{\partial T}{\partial t}}_{\Delta \text{ enthalpy}} = \underbrace{\rho\frac{\partial}{\partial m}\left(\rho r^4 k \frac{\partial T}{\partial m}\right) - \sum_{i=1}^{N} \rho^2 r^2 c_{p,i} u_{d,i} Y_i \frac{\partial T}{\partial m}}_{\text{diffusion}} - \underbrace{\sum_{i=1}^{N} h_i \dot{\omega}_i}_{\text{heat release}} \quad (2)$$

transformation to mass-weighted Lagrangian coordinates $(r, t) \rightarrow (m, t)$:

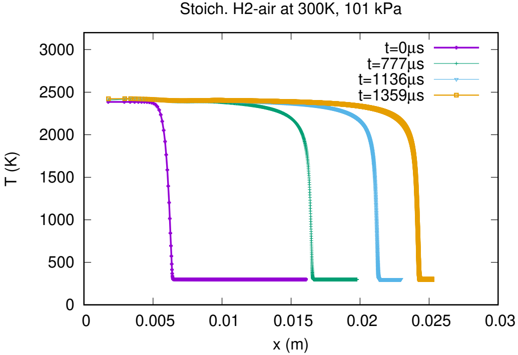
$$m(r, t) = \int_{r=0}^{r} \rho r^2(r, t) dr \quad (3)$$

Numerical Method:

- Written in C/C++
- Low Mach number approximation ($\nabla p \approx 0$) [Paolucci, 1982]
- Incorporates Cantera libraries [Goodwin et al., 2018]
- Detailed USC-Mech II mechanism (10 species, 28 reactions) [Davis, 2005]
- Explicit upwind differencing on advection-like terms
- Explicit central differencing on 2nd order diffusion term
- Implicit integration of reaction terms using Sundials CVODE libraries [Cohen and Hindmarsh, 1996]
- Parallelized for shared memory using Open-MP [Dagum and Menon, 1998]
- Run on HPC, using 16 CPUs per simulation

Numerical Method:

- Resolved on 5000 computational cells per simulation
- Domain size: $r \geq 24\text{mm}$
- Spatial resolution corresponds to $\Delta r \leq 4.8\mu\text{m}$
- Ma evaluated from $8\text{mm} \leq R_f \leq 24\text{mm}$



Obtaining the Marktein number:

Markstein length and flame speed in burned products:

$$S_b = S_b^0 - L_b \cdot \kappa, \quad (4)$$

Stretch rate is $\kappa = 2\frac{S_b}{R_f}$, R_f is the flame radius, and S_b is given by $S_b = \frac{dR_f}{dt}$. Integrating (4) w.r.t.t gives

$$S_b^0 \cdot t = R_f + 2L_b \cdot \ln\left(R_f\right) + C_{st}, \quad (5)$$

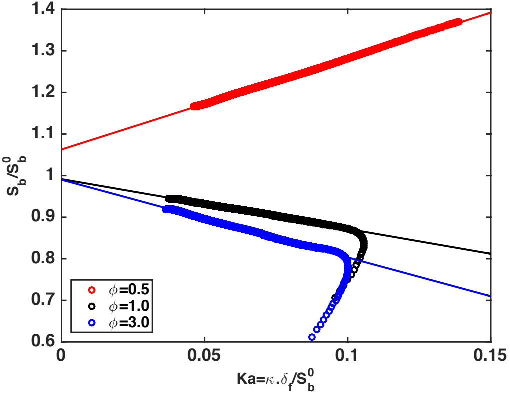
S_b^0 and L_b in burned products are found using least-square fitting and related to S_u^0 and L_u through expansion ratio $(\sigma = \rho_u/\rho_b)$ Finally, the Markstein number is

$$Ma_u = \frac{L_u}{\delta_f}, \quad (6)$$

where δ_f is the unstretched flame thickness.

Extrapolation model:

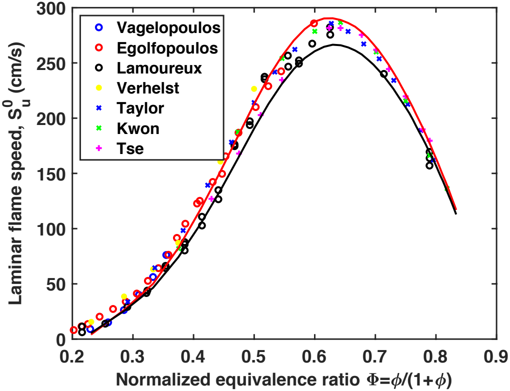
- Lean flames have −ve Ma, while other cases have +ve Ma
- Extrapolation to zero-stretch is consistent ($S_b/S_b^0 \rightarrow 1$)



Points: Simulation; Lines: Extrapolation model.

Unstretched flame speeds:

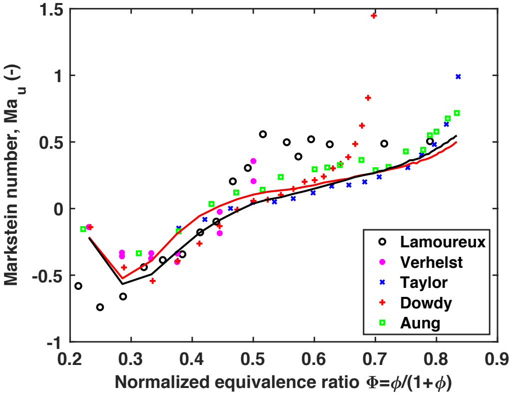
- Experimental S_u^0 captured within 5% mean absolute error
- 40-45 % discrepancies for very lean



Red: Mixture-averaged transport; Black: Multi-component.

Markstein numbers:

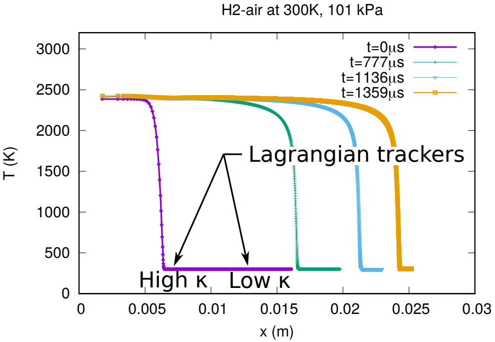
- Ma for lean mixtures captured well
- Discrepancies for rich mixtures
- USC-II well suited for FA and DDT in lean mixtures



Red: Mixture-averaged transport; Black: Multi-component.

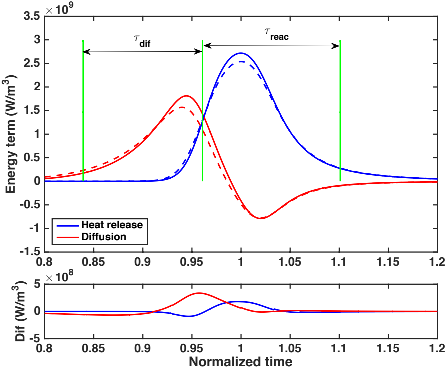
Lagrangian particle dynamics:

- Lean: $\phi = 0.5$, $Ma = -0.15$
- Rich: $\phi = 3.0$, $Ma = +0.15$
- Lagrangian trackers placed to measure dynamics for $Ka = 0.075$ and $Ka = 0.05$ ($Ka = \kappa\delta_f / S_b^0$)



Lagrangian particle dynamics:

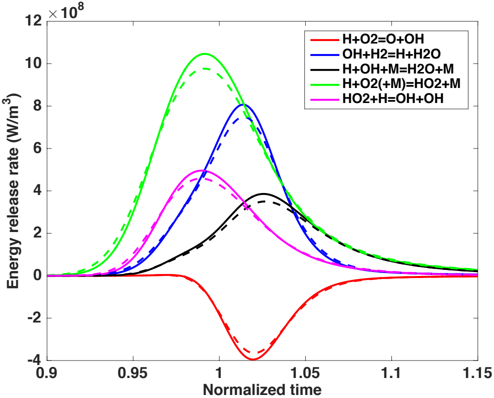
- Low Karlovitz (Ka) number has ↑ initial heat diffusion
- High Ka has ↑ heat diffusion at end of τ_{diff}
- $-$ve Ma has ↑ heat release as expected



($\phi = 0.5$, $Ma = -0.15$) Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Lagrangian particle dynamics:

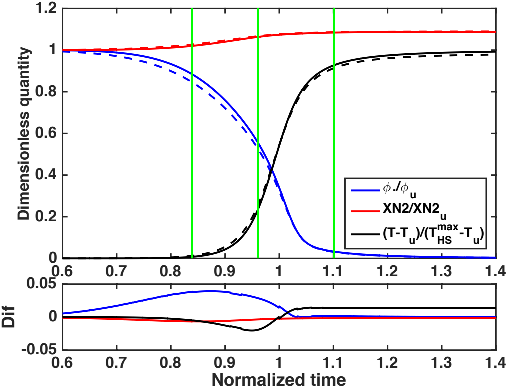
- Dominant reaction pathways the same for both Ka
- Low Ka initially has ↑ energy release rates
- High Ka overall has ↑ energy release rates



Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Lagrangian particle dynamics:

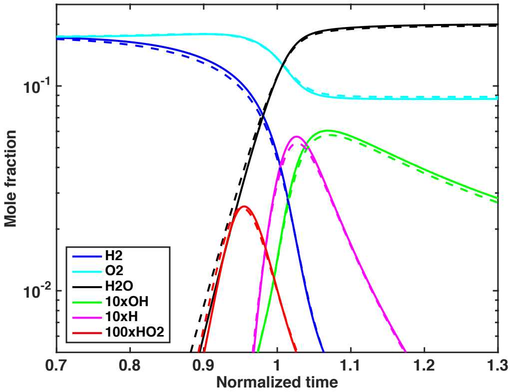
- Lower Ka leads to faster drop in ϕ due to $\uparrow$ diffusion of hydrogen (before chemistry), vice-versa



Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Lagrangian particle dynamics:

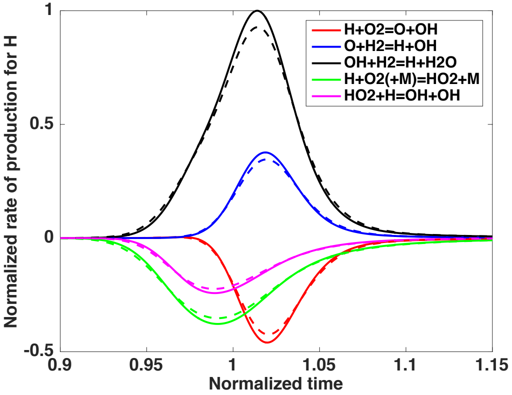
- Drop in ϕ evident by drop in $\mathrm{H_2}$



Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Rate of production of H:

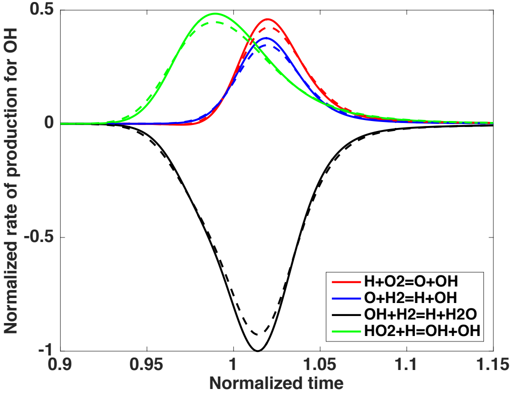
- ↑ Ka ultimately leads to ↑ ROP of all reactions



Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Rate of production of OH:

- $H + O_2 + (M) \rightleftharpoons HO_2 + (M)$ first, then $HO_2 + H \rightleftharpoons OH + OH$ reactions important for lean flames



Solid: $Ka = 0.075$; Dashed: $Ka = 0.05$

Conclusions:

- Untstretched laminar flame speed captured well
- Discrepancies observed for fuel-rich Ma
  - Can lead to inaccurate prediction of stability in rich flames
  - Implications on simulating flame acceleration and DDT

Conclusions:

- For lean mixtures:
  - Diffusion of H2 is slower at high stretch rate (κ)
  - Less lean flame
  - $\uparrow$ reactivity and flame speed w.r.t. stretch rate
- For rich mixtures:
  - Diffusion of H2 is faster at high stretch rate
  - More lean flame
  - $\uparrow$ reactivity w.r.t. stretch rate (despite $+$ve Ma)

Acknowledgement

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