Effects of Kinetics on Ignition of Hydrogen Jets

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Motivation

- Hydrogen as a viable alternative fuel source
- High pressurized hydrogen might lead to an accidental explosion
- Ignition: safety concern
- Rezaeyan (2011): Role of Lewis number for single step kinetics of hydrogen jet ignition

Background Information

- Astbury and Hawksworth (2007) postulated mechanisms:
  - Reverse Joule-Thompson effect, electrostatic ignition, diffusion ignition, sudden adiabatic compression, and hot surface ignition.

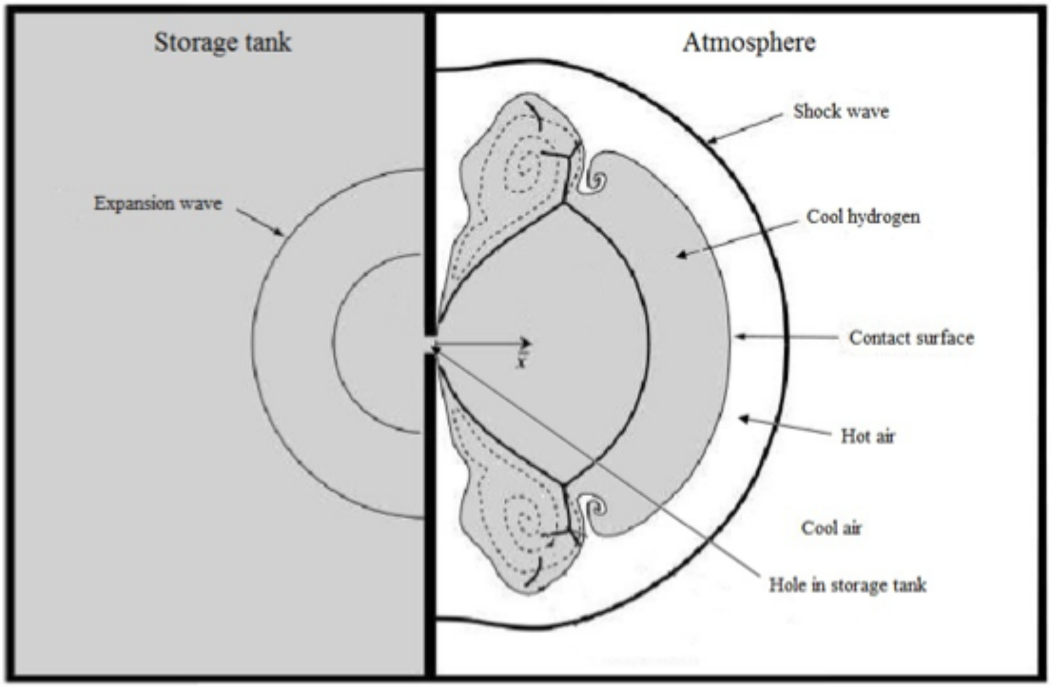
- Wolanski and Wojcicki (1973) first observed that in hydrogen leaks, auto-ignition can occur

- High pressure leak:

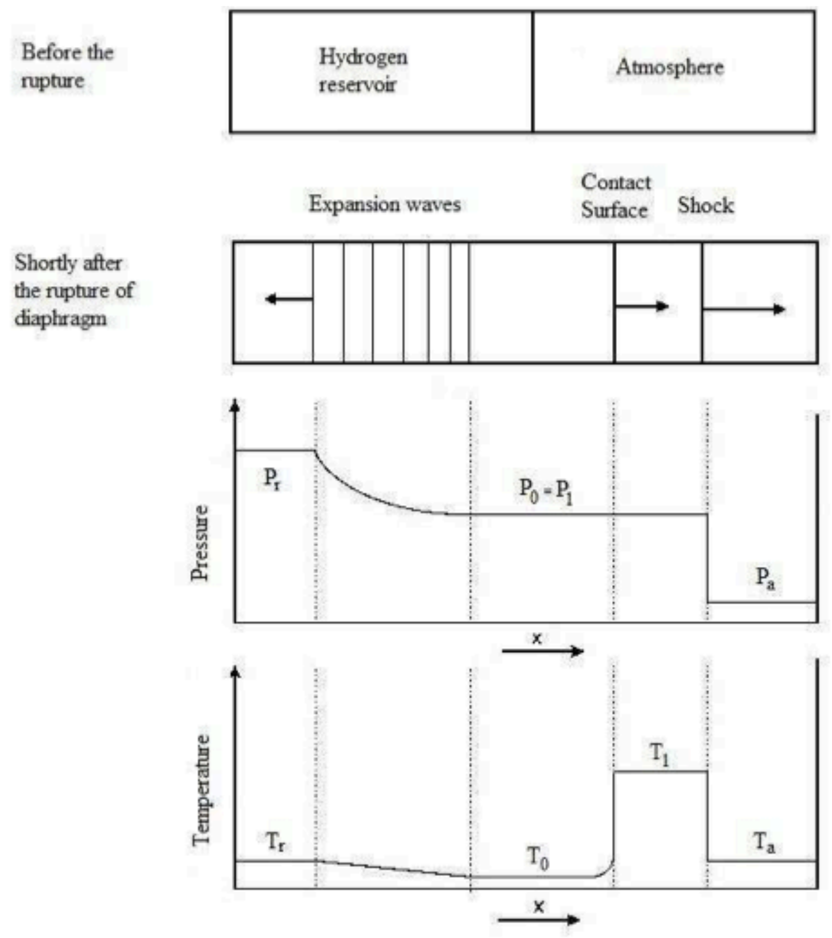
  - Pressurized gas discharges into surrounding atmosphere, driving a shock wave in front of the jet
  - Shock is followed by a contact surface separating hot air from hydrogen (cooled by expansion)
  - Mixing along contact surface may lead to ignition

Physical Model

- Early stages similar to standard shock tube problem
- Radulescu (2007)



Physical Model



Physical Model

- Taken as 1-D
  - Diffusion thickness small compared to curvature radius
- Expansion term added to the shock tube model
- Ideal gas, constant specific heats
- All initial conditions are known
- Expansion rate is known in time

Formulation

- Chemical Kinetics:
  - Start with arbitrary chemical reaction equation
  - Arrhenius law used to determine rates of reaction

$$\kappa_j(T) = A_j(T)e^{-E_{aj}/(RT)}$$

- 8 Species are considered in H_2-O_2 oxidation
  - H, O, H_2, O_2, OH, H_2O, HO_2, H_2O_2

Formulation

- Conservation laws:
  - Mass, energy and species conservation
- Heat and mass diffusion
  - Fourier’s Law of conduction
  - Fick’s law of diffusion
- Lewis Numbers stays constant
- Boundary conditions: Shock tube relations
  - Density, pressure and temperature will drop due to expansion

Assumptions

- Key Processes: Reaction, Diffusion, Expansion
- Mach numbers small
  - Momentum conservation→ pressures approximately uniform
- Diffusive length small
  - Expansion is spatially uniform

Frozen Flow

- Absence of chemistry
- Conservation equations include: transient diffusion, advection, expansion
- Time is scaled such that, initially, there is little chemistry
    - Reduced to diffusion problem

Frozen Flow

- Assume diffusivities are inversely proportional to the square of density
  - Mass-weighted spatial coordinate

$$z = (\rho f)^{-1/2} \int_0^y \varrho dy$$

- Introduce similarity parameter

$$\eta = z/(2\sqrt{\tau}):$$

  - System reduces to one independent parameter
  - Except expansion term (non-homogeneous)

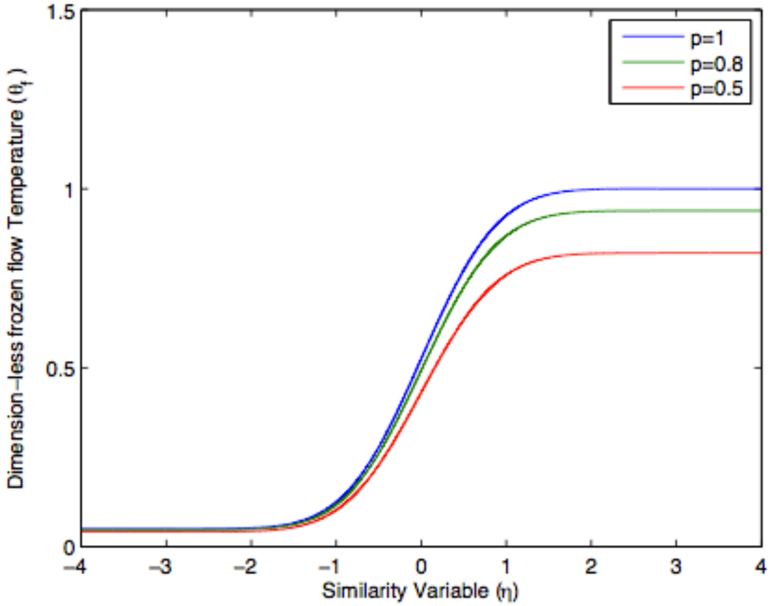
Frozen Flow

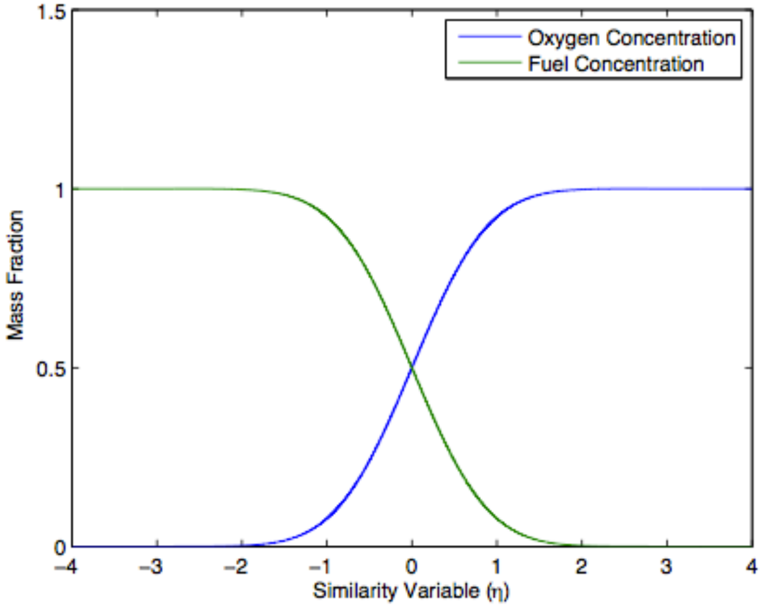
- Solution is self-similar expressed using error functions
- Solution to Frozen Flow

$$\begin{aligned}
y_{H_2fr} &= \tfrac{1}{2}\left[1 - erf(\eta\sqrt{Le_{H_2}})\right] \\
y_{O_2fr} &= \tfrac{1}{2}\left[1 + erf(\eta\sqrt{Le_{O_2}})\right] \\
y_{isfr} &= 0 \\
\theta_{fr} &= 1 + \tfrac{1}{2}(1 - \Delta_\theta)(erf(\eta) - 1) \\
\varrho_{fr} &= 1/\theta_{fr}
\end{aligned}$$

Frozen Flow

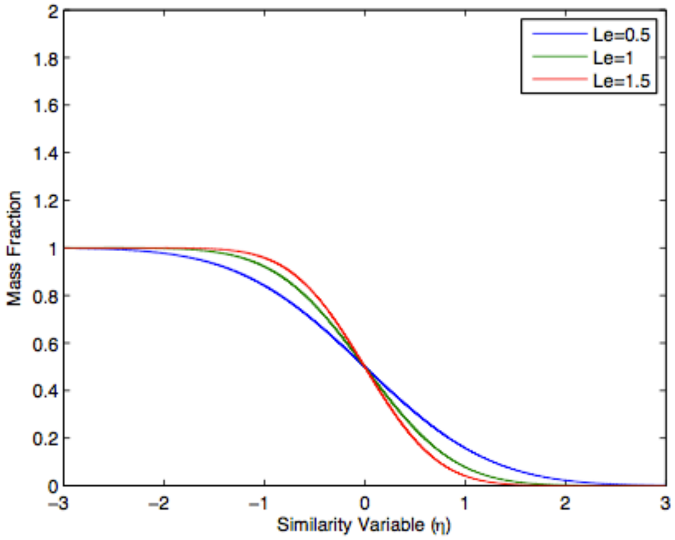
- Results

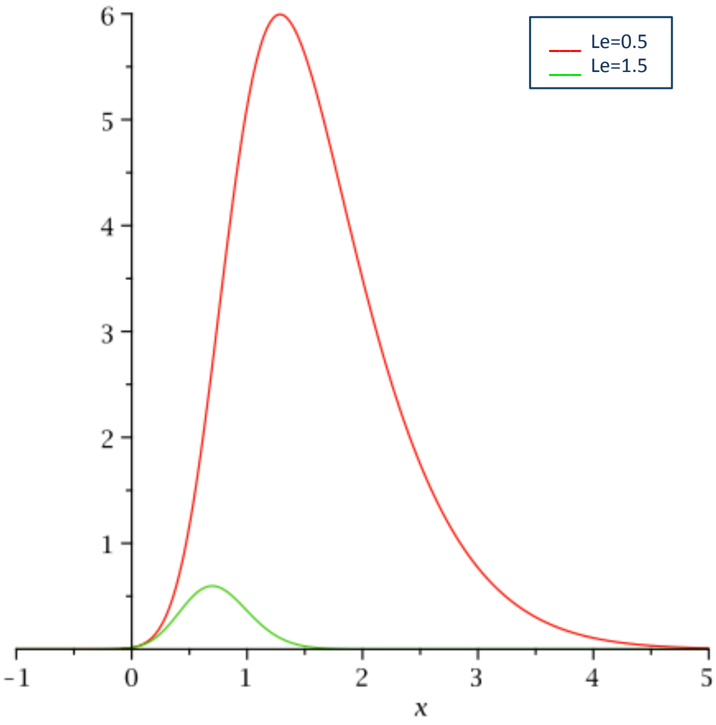




Frozen Flow

- Results



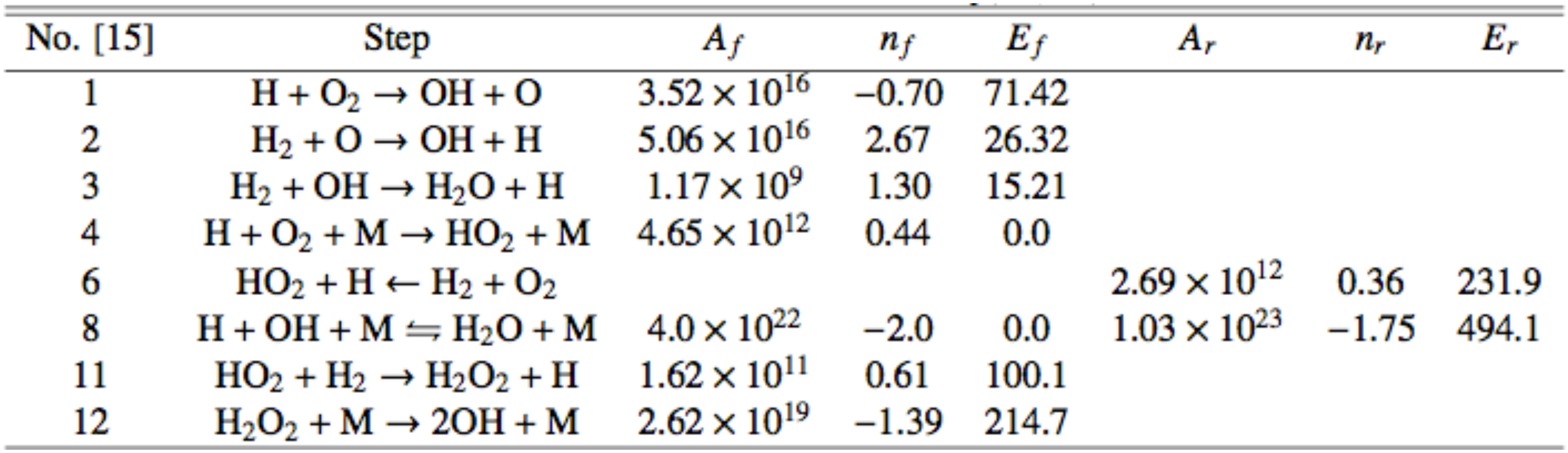


Perturbation

- Perturbation added to frozen flow
  - Accounts for small effect of chemistry
- Rate magnitudes
  - Initiation: slow
  - Termination: fast
  - Other steps: intermediate rate values

Chemical Kinetics

- San Diego Mechanism (Boivin 2011)
  - 21 reversible elementary reactions
  - Reduced to 12



No. [15]	Step	A_f	n_f	E_f	A_r	n_r	E_r
1	$H + O_2 \rightarrow OH + O$	3.52×10^{16}	−0.70	71.42			
2	$H_2 + O \rightarrow OH + H$	5.06×10^{16}	2.67	26.32			
3	$H_2 + OH \rightarrow H_2O + H$	1.17×10^{9}	1.30	15.21			
4	$H + O_2 + M \rightarrow HO_2 + M$	4.65×10^{12}	0.44	0.0			
6	$HO_2 + H \leftarrow H_2 + O_2$				2.69×10^{12}	0.36	231.9
8	$H + OH + M \leftrightharpoons H_2O + M$	4.0×10^{22}	−2.0	0.0	1.03×10^{23}	−1.75	494.1
11	$HO_2 + H_2 \rightarrow H_2O_2 + H$	1.62×10^{11}	0.61	100.1			
12	$H_2O_2 + M \rightarrow 2OH + M$	2.62×10^{19}	−1.39	214.7			

Perturbation

- Conservation of species k:

$$\frac{\partial y_k}{\partial t} - \frac{\eta}{2t}\frac{\partial y_k}{\partial \eta} - \frac{1}{4tLe_k}\frac{\partial^2 y_k}{\partial \eta^2} = \frac{1}{\rho}\Sigma\omega_{ijk}$$

- Rates are written as:

$$\omega_{ik} = \pm C y_i^m y_j^n T^a \exp\frac{E}{RT}$$

  - Arrhenius

- Perturbations are introduced of order $\varepsilon = y_{il}/y_{ij} \ll 1$

- Time is scaled by $1/y_{ij}$

Perturbation

- *Conservation of species*

$$\frac{\partial y_k^{(1)}}{\partial t} - \frac{\eta}{2t}\frac{\partial y_k^{(1)}}{\partial \eta} - \frac{1}{4Le_k t}\frac{\partial^2 y_k^{(1)}}{\partial \eta^2} = \frac{1}{\rho}\Sigma_i a_{ik} y_i^{(1)} + \frac{s}{\rho} + \frac{b}{\rho} y_H^{(1)} y_{OH}^{(1)}$$

- Non linear
- Equations are coupled through the first and last term on the r.h.s.

Numerical Solution

- Splitting up equation: stiff and diffusion

$$\frac{\partial y_k^{(1)}}{\partial t} - \frac{\eta}{2t}\frac{\partial y_k^{(1)}}{\partial \eta} - \frac{1}{4Le_k t}\frac{\partial^2 y_k^{(1)}}{\partial \eta^2} = \frac{s}{\rho}$$

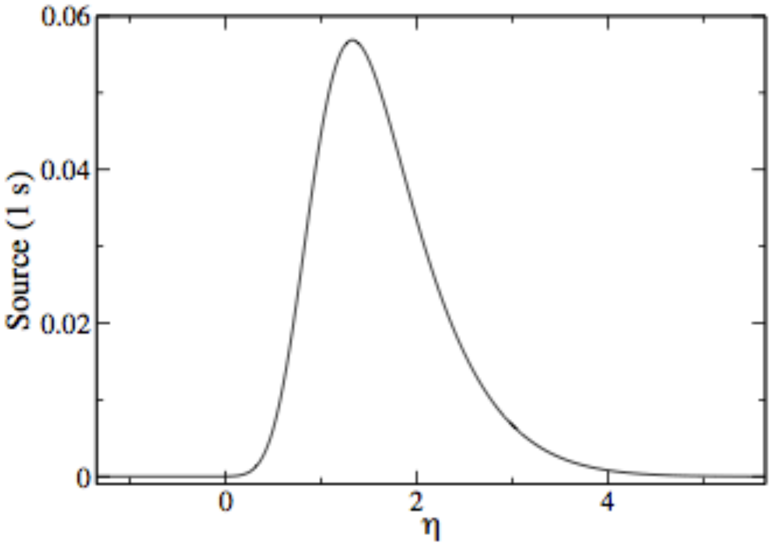
$$\frac{\partial y_k^{(1)}}{\partial t} = \frac{1}{\rho}\Sigma_i a_{ik} y_i^{(1)}$$

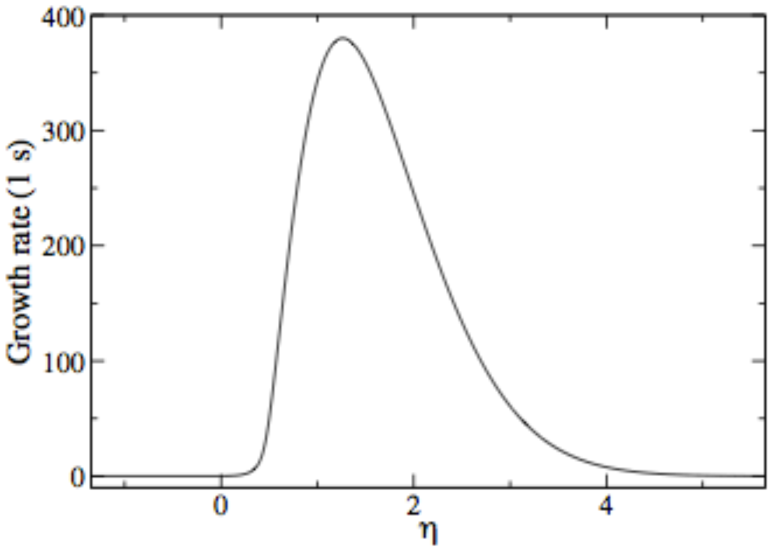
$$\frac{\partial y_k^{(1)}}{\partial t} = \frac{1}{\rho}\frac{b}{\rho} y_H^{(1)} y_{OH}^{(1)}$$

- Stiff: project upon eigenmodes; termination: backward integration
- Diffusion: source as tY(η) + hermite polynomials for homogeneous part

Results

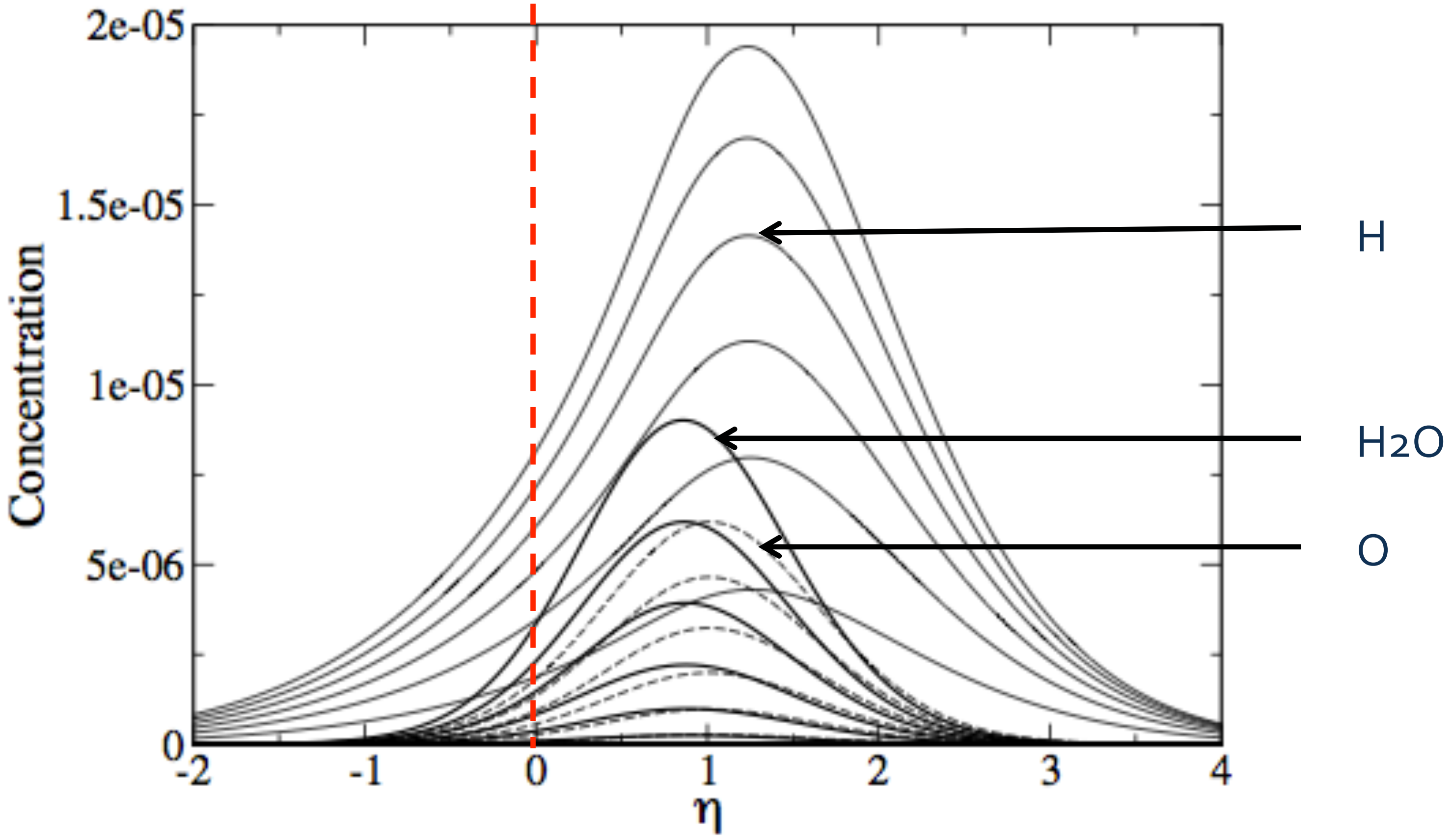
- Source and single positive eigenvalue of matrix A vary with η
- Initiation and chain branching occurs well into the warm air region





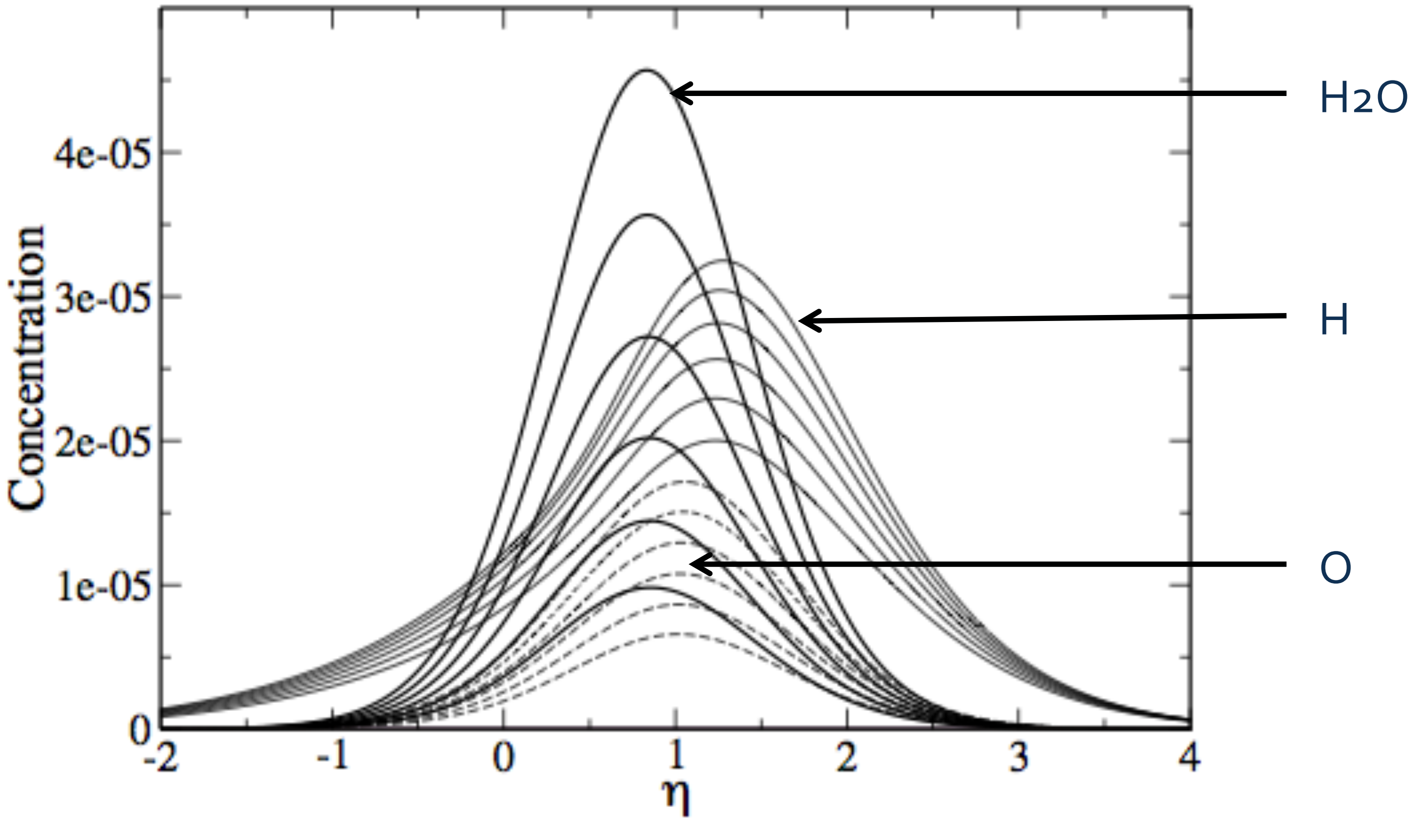
Results

- Early times (0.2 to 2.0 ms)



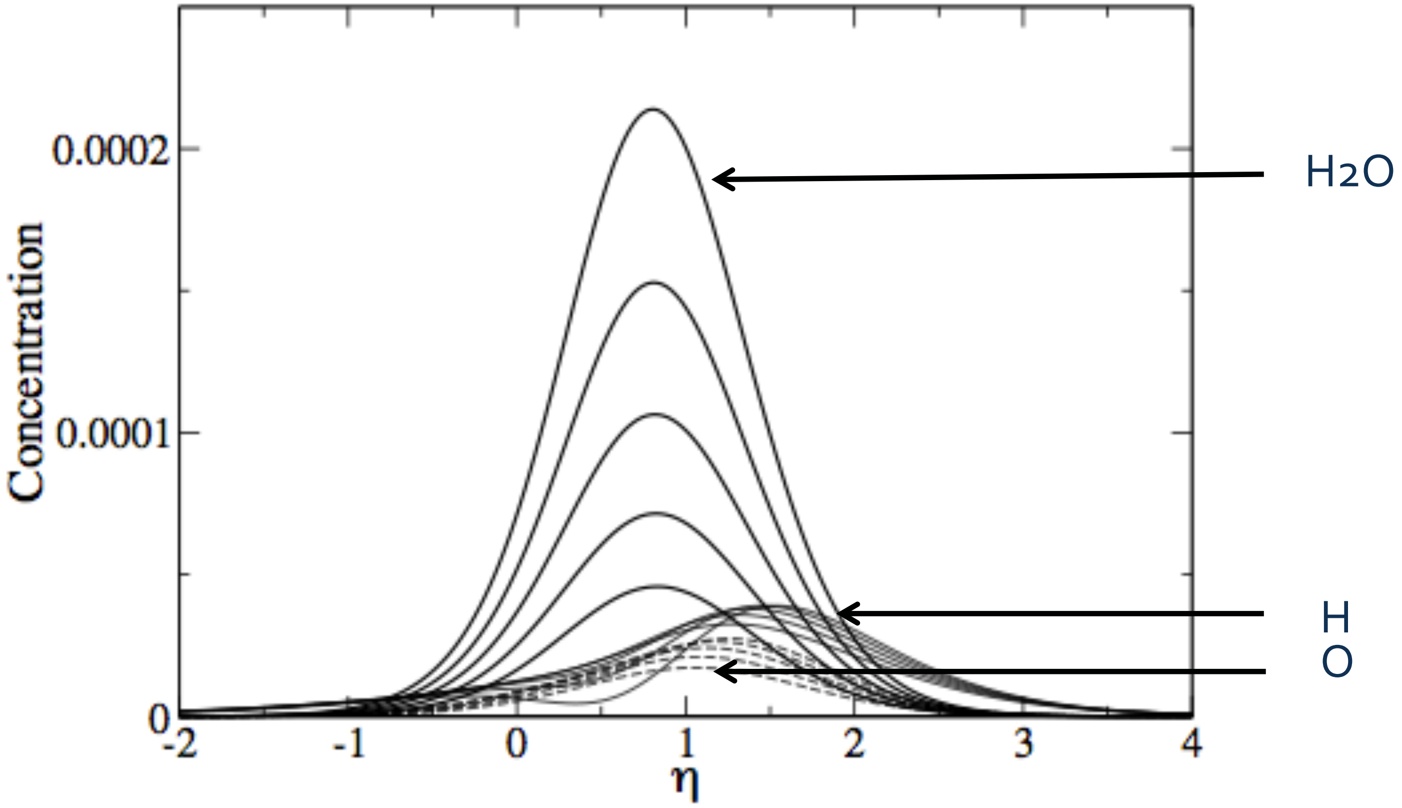
Results

- Intermediate times (1.25 to 2.5 ms.)



Results

- Late times (2.5 to 4.5 ms)



Analysis of Results

- At later times initiation is no longer important
- Water production increases with time
  - Water concentration at its peak now exhibits faster growth than the species released by initiation
- As the perturbation values become large, the assumption that temperature changes have negligible effects will no longer be valid
- Lewis number plays key role in initiation
  - Hydrogen diffuses much more quickly than heat

Conclusion

- Chemical reaction + diffusion problem
  - Numerical solution (split algorithm)
- Results presented for San Diego mechanism
  - Not expected to be very different for other kinetic schemes
- Importance of the Lewis number confirmed from previous study
  - Initiation, which is slow and stiff, occurs well within the warm air region
  - Le<1: More likely to ignite