Subgrid-Scale Reaction Modeling Applied to Turbulent Combustion Simulations

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Heptane Pool Fire
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Objectives

CFD Simulations of
Combustion Scenarios

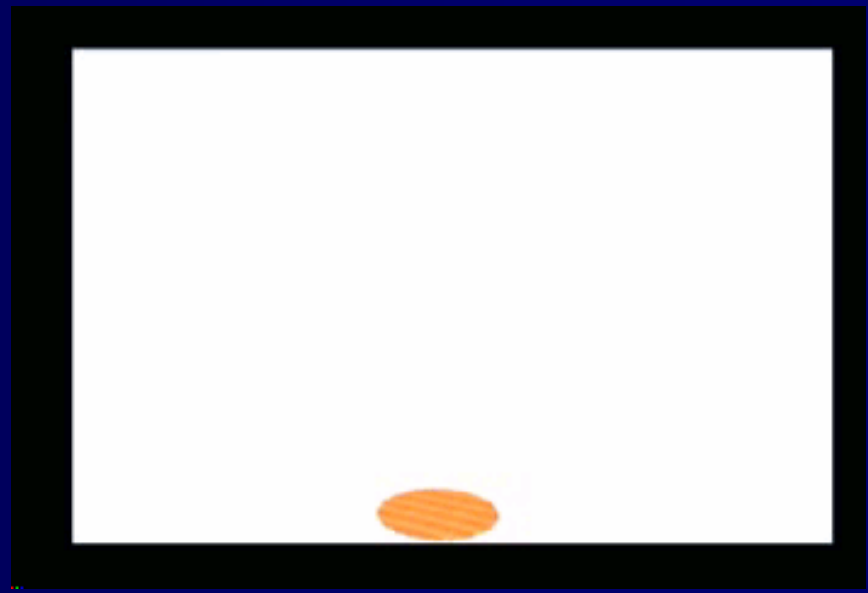
Motivation

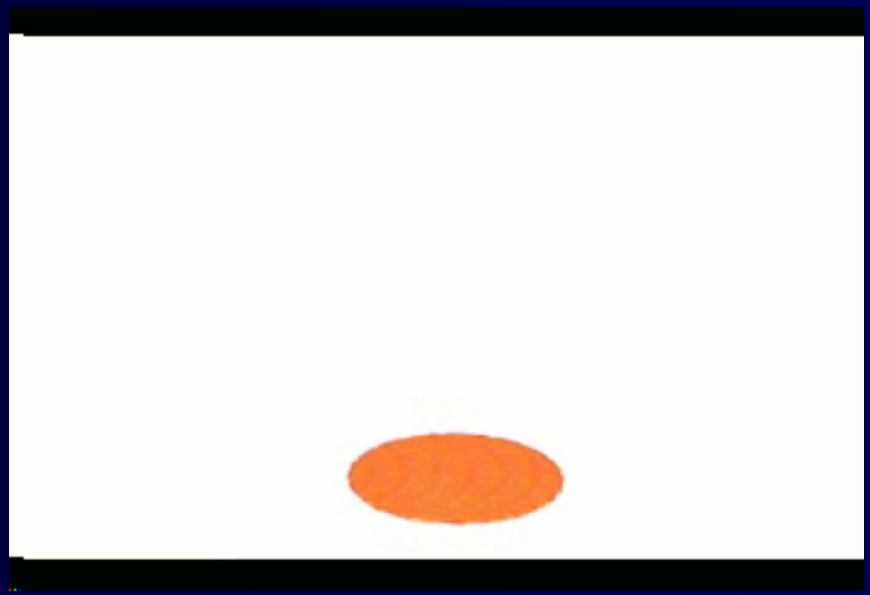
- Heat Fluxes - Temperatures
- Emissions - Soot

N-pentane pool fire
25 m dia., 4 ms exposure
Courtesy of Schonbucher
Institut fur Technische Chemie I der Universitat Stuttgart

Arches Fire Simulations

- 10 m. dia. Heptane pool fire
- 30^3 m domain, 150^3 nodes
- 125 processors at LANL ASCI Blue Mountain (Nirvana)
- 24 hrs clock time (3000 CPU)
- 10 sec. simulation

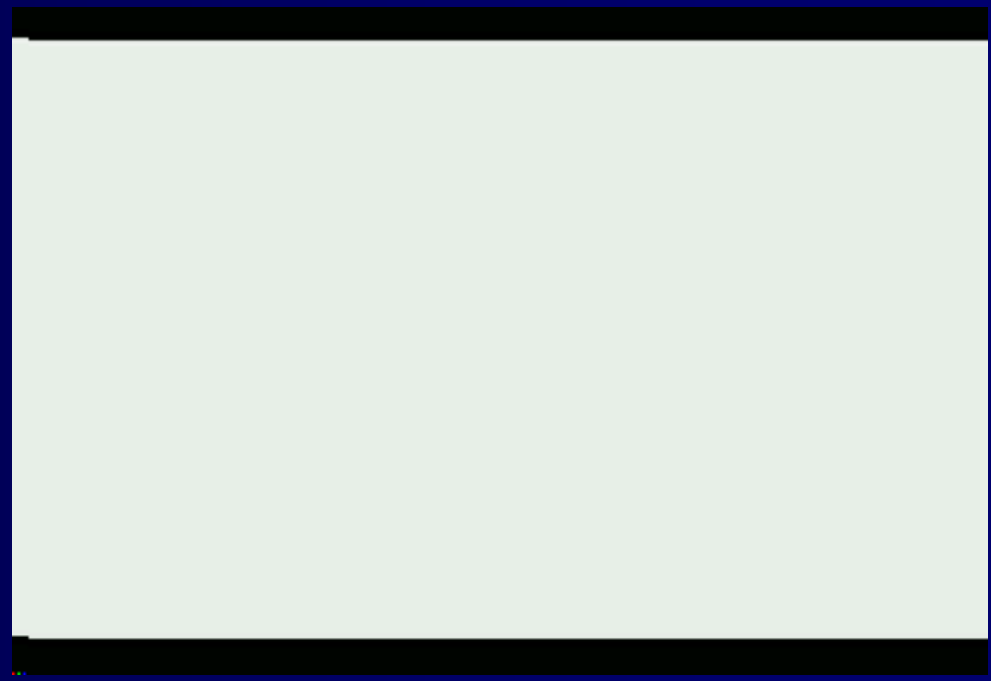




- 10 m. dia. Heptane pool fire
- 70^3 m domain, 150^3 nodes
- 500 processors at LANL ASCI Blue Mountain (Nirvana)
- 12 hrs clock time (6000 CPU)
- 8 sec. simulation

Arches Fire Simulations

- 10 m. Heptane pool fire
- 30^3 m domain
- 300^3 nodes
- 1000 processors at LANL ASCI Blue Mountain (Nirvana)
- 36 hrs clock time (36,000 CPU)
- 8 sec. simulation



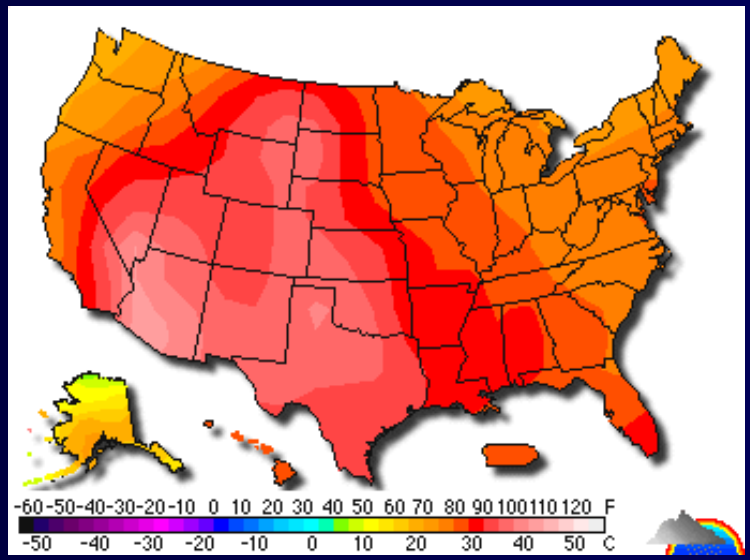
How Do We Simulate a Fire?

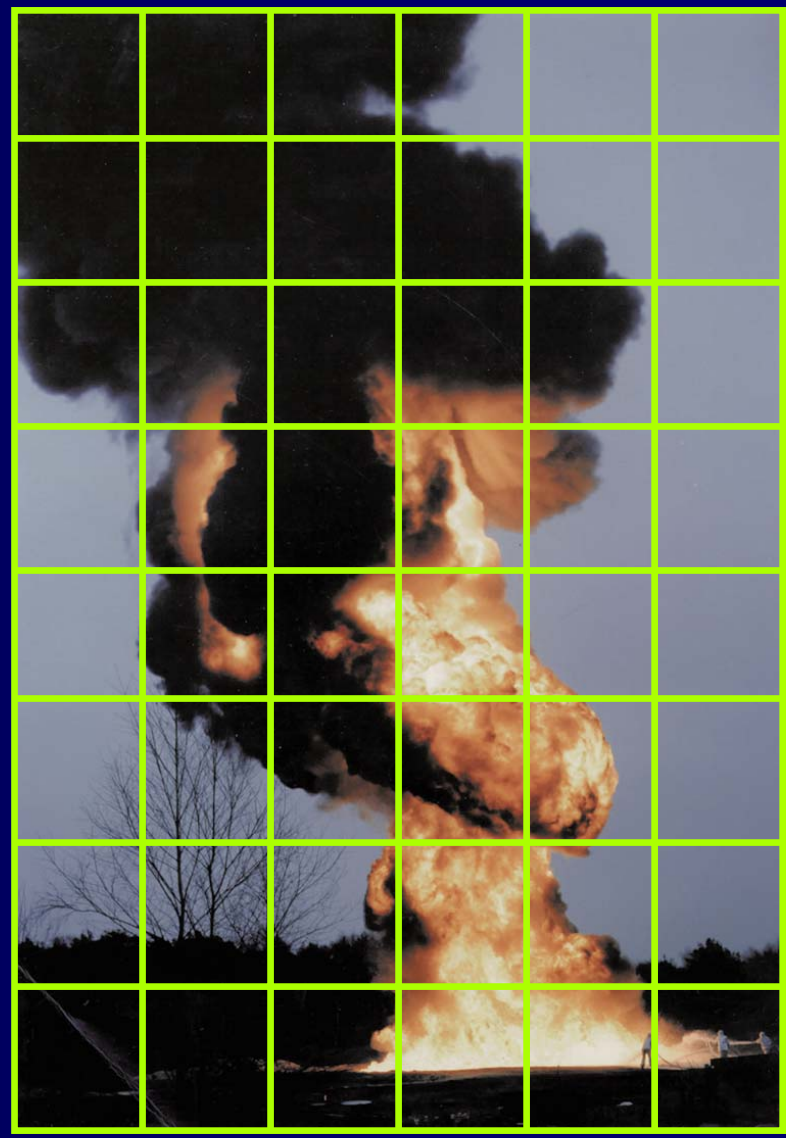
Apply a Computational Mesh

(like Rubik's Cube)

- CFD - Conserve Mass, Momentum, and Energy
- Reactions - Conserve Species

Weather Map Example





N-pentane pool fire
25 m dia., 4 ms exposure
Courtesy of Schonbucher
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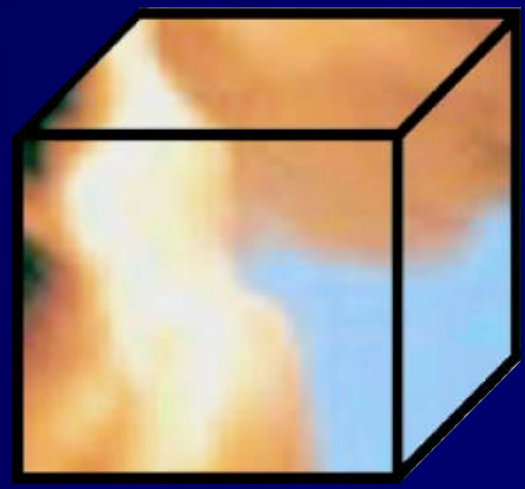
Subgrid Scale Reaction Model

Gas Phase:
LLNL C7 Mechanism

- 160 species
- 1534 elementary rxns



Solid Phase: soot to be discussed

SGS Rxn Model

Given η_i and π_j, a reaction model calculates

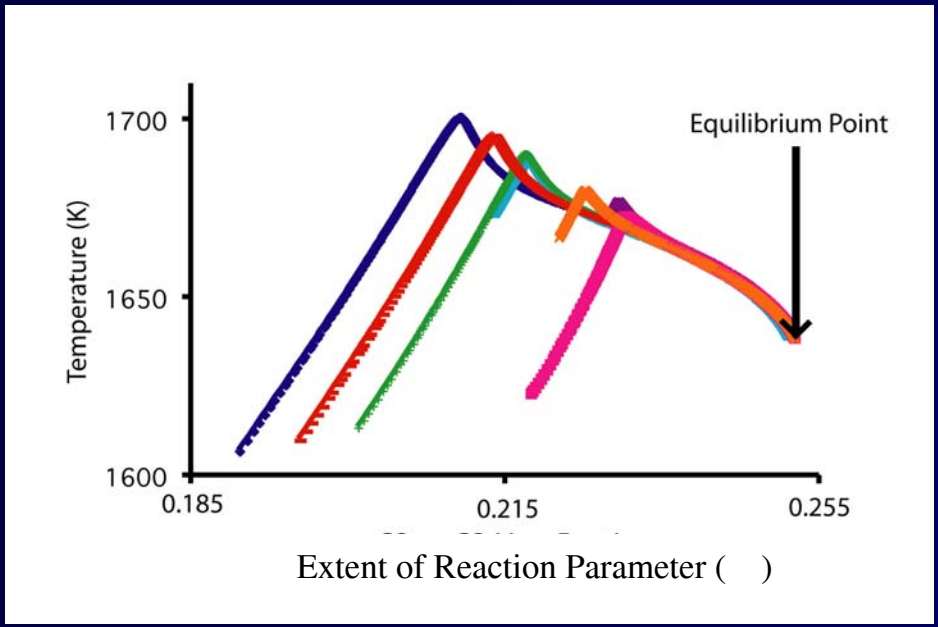
$\varphi = [y_k, r_k, T, \rho, \ldots]$

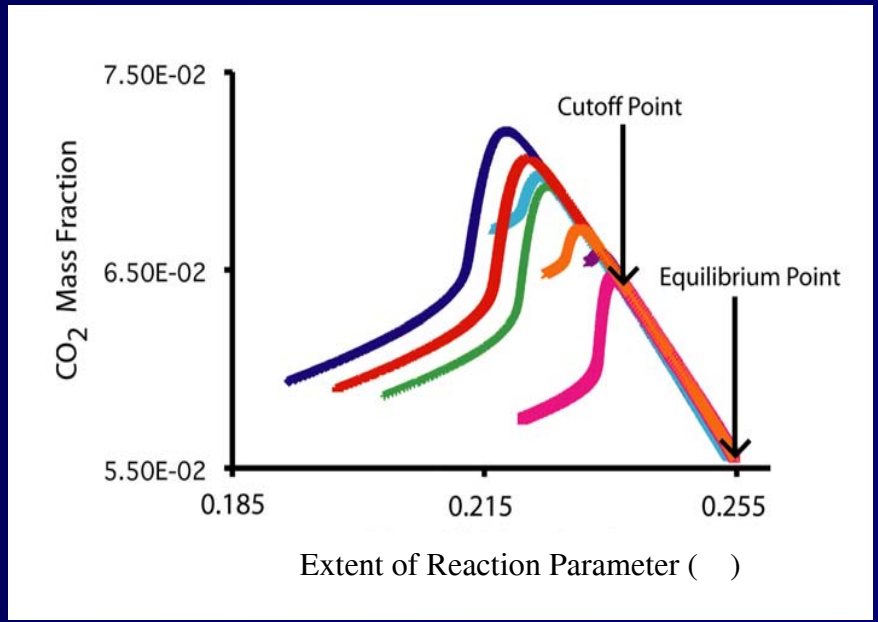
Rxn Model Criteria

1. Non-equilibrium effects
2. Molecular transport
3. Minor/transient species

LDM Concept (Gas Phase)

Intrinsic Lower Dimensional Manifold (ILDM)



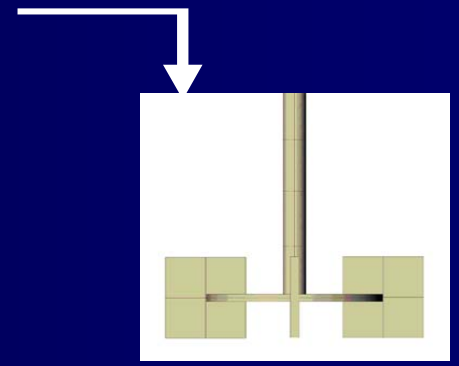


For the LLNL heptane mechanism,
the degrees of freedom is decreased from 160 to 3!

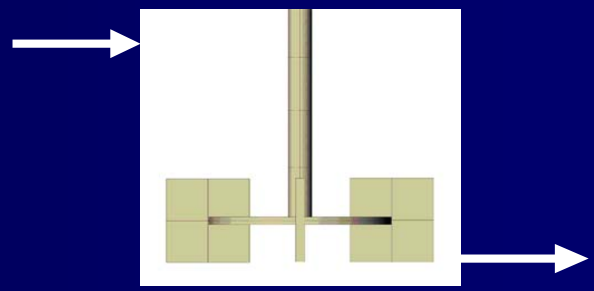
Thus CFD requires only mixture fraction, enthalpy, and extent of reaction transport.

LDM Reaction Models

ILDM
(instantaneous mixing)

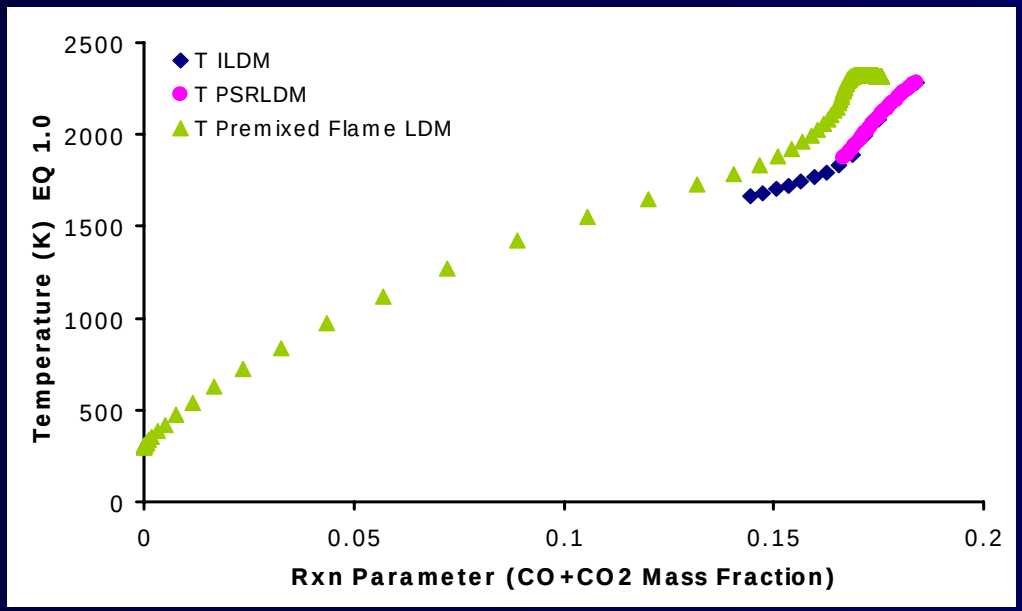


PSR LDM (flow effects)

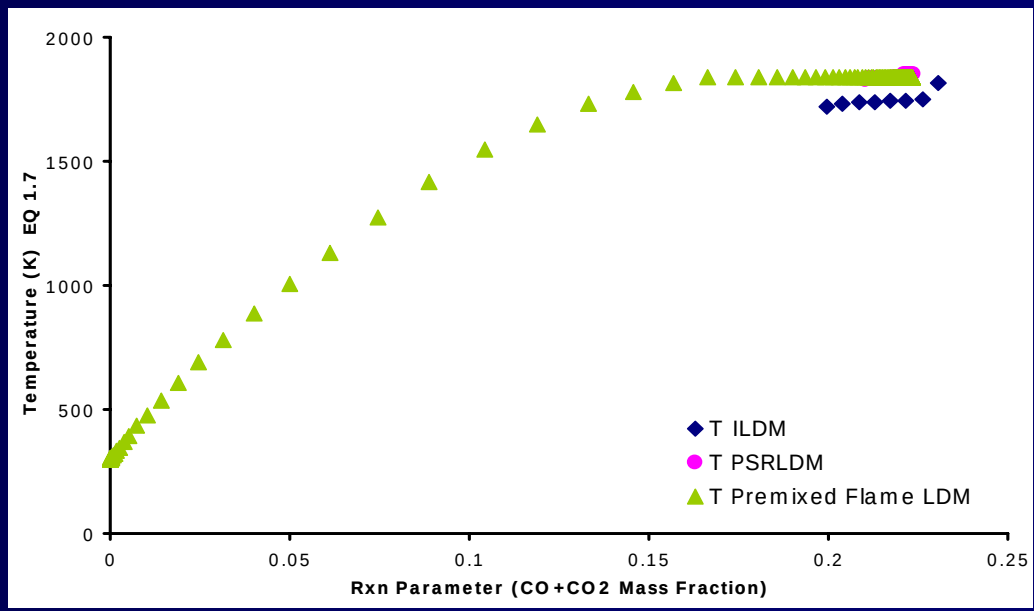


Premixed Flame LDM
(molecular diffusion)

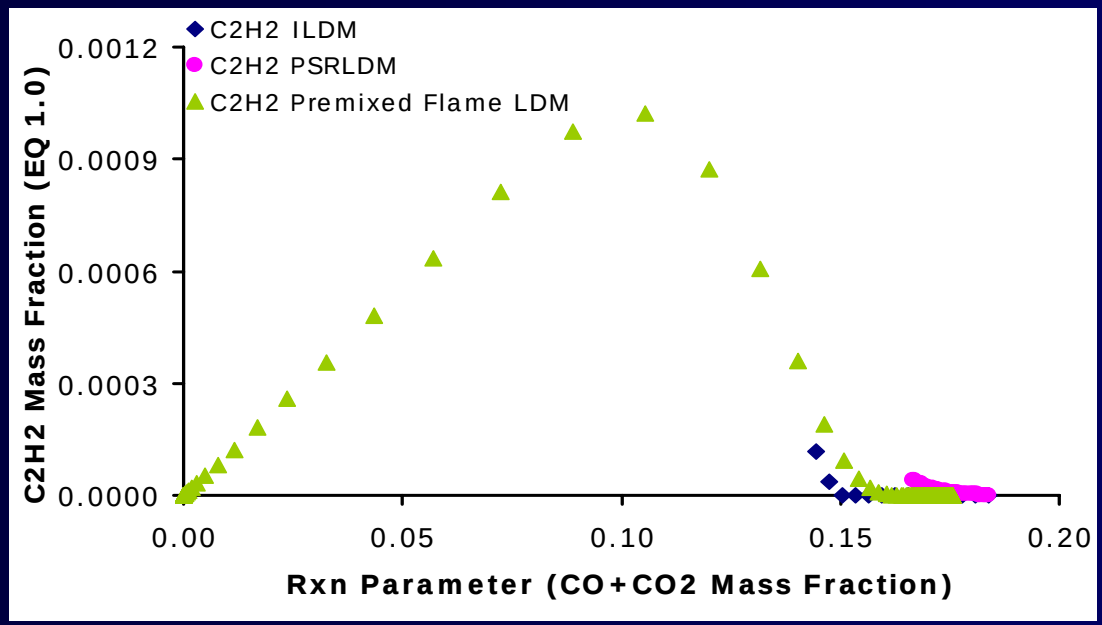
Comparison of LDM Models



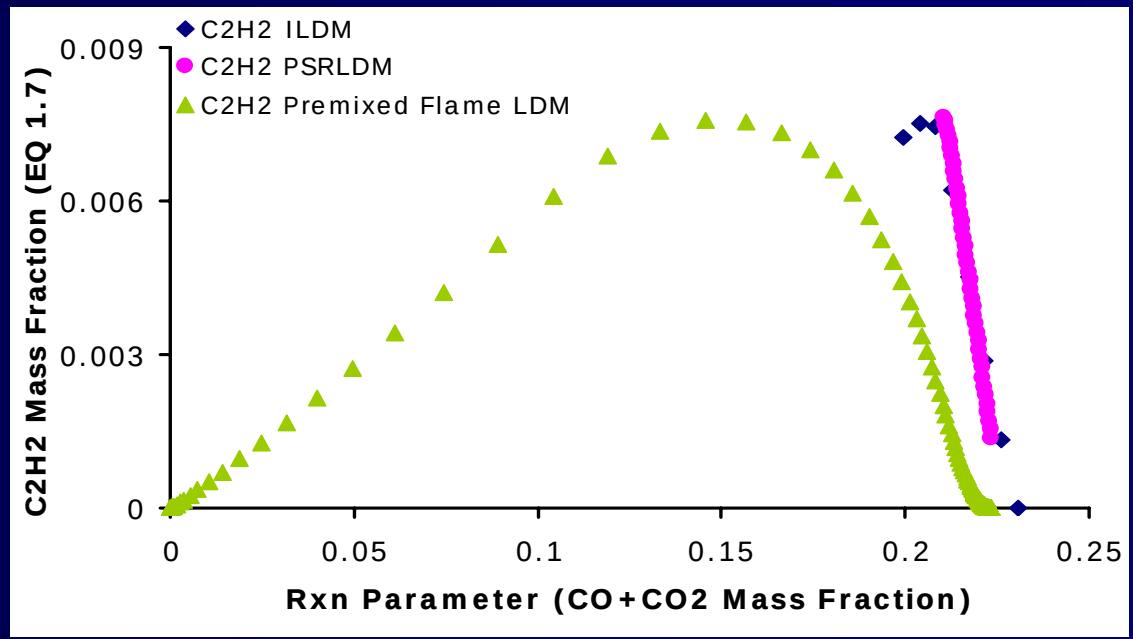
Temperature



Comparison of LDM Models



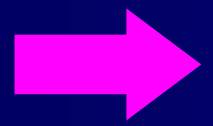
C_2H_2
Soot Precursor



Soot Incorporation (Solid Phase)

Leung soot formation and oxidation model

1. $C_2H_2 \rightarrow 2C(s) + H_2$ [Nucleation]
2. $C_2H_2 + nC(s) \rightarrow (n+2)C(s) + H_2$ [Surface Growth]
3. $C(s) + 1/2O_2 \rightarrow CO$ [Oxidation]
4. $nC(s) \rightarrow C_n(s)$ [Agglomeration]



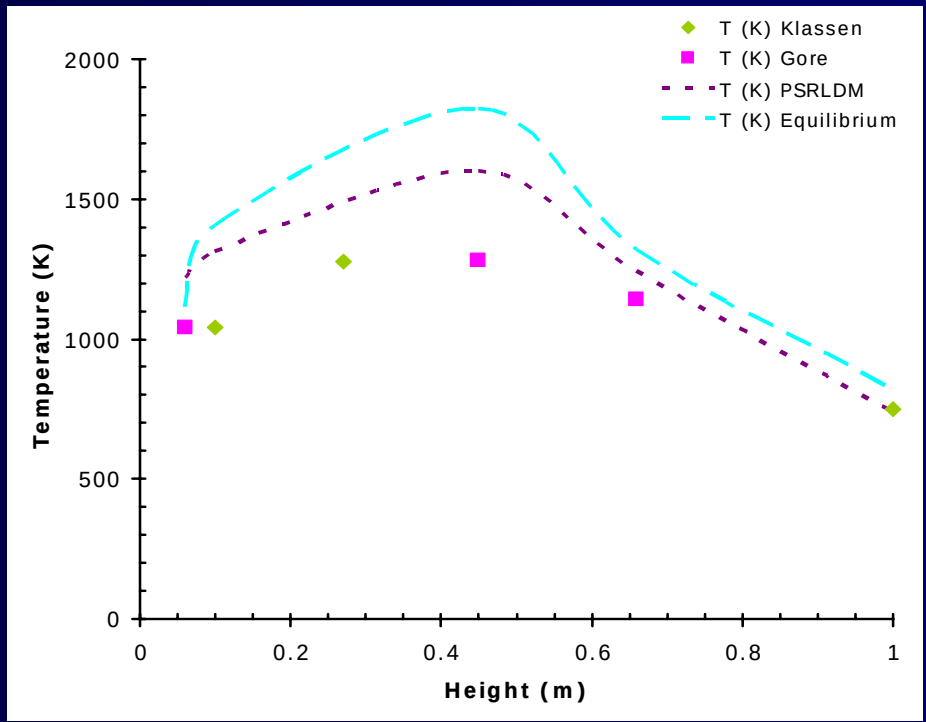
- Soot Mass
- Soot Density

LES Summary

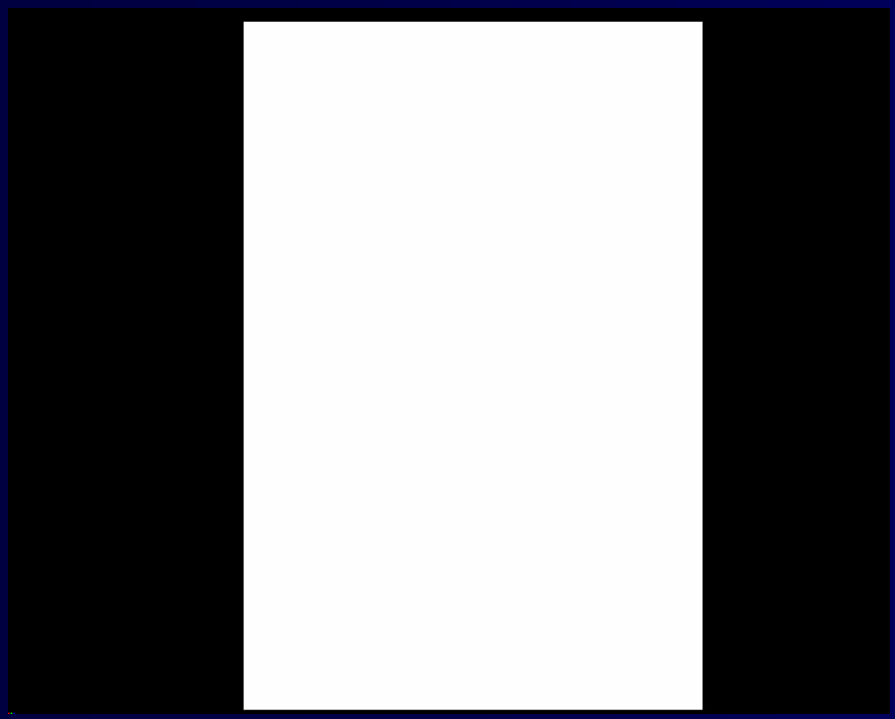
- Mass
- Momentum
- Energy
- Mixture fraction
- Extent of reaction
- Soot mass fraction
- Soot particle # density

30 cm Heptane Pool Fire Simulation

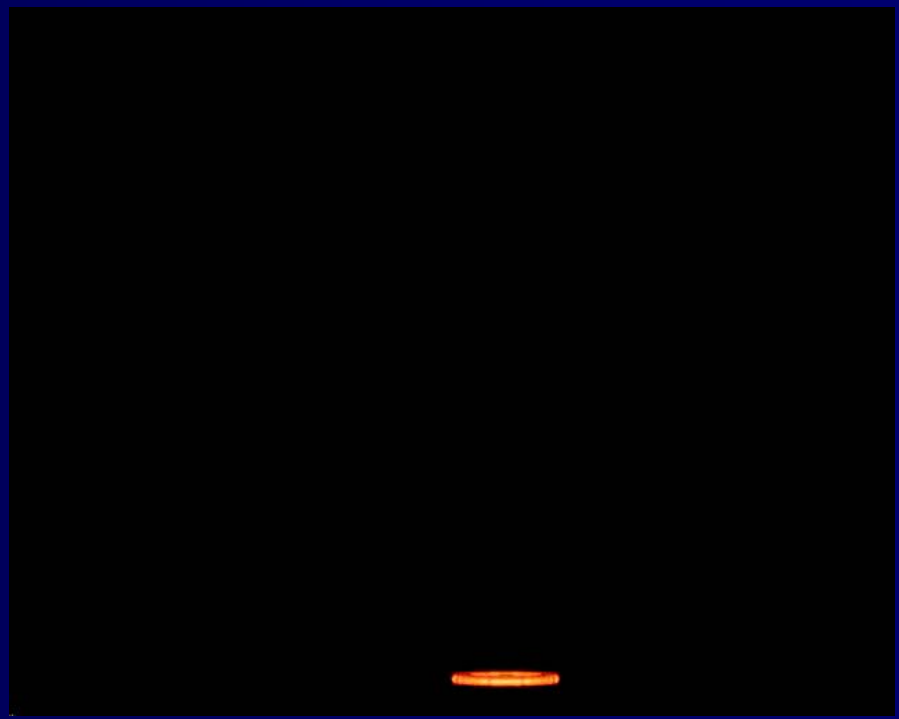
- 3-D LES
- 1 m^3 domain, 60^3 mesh
- 32 processors, 2-3 days CPU time
- 6 sec simulation time



Soot Volume Fraction



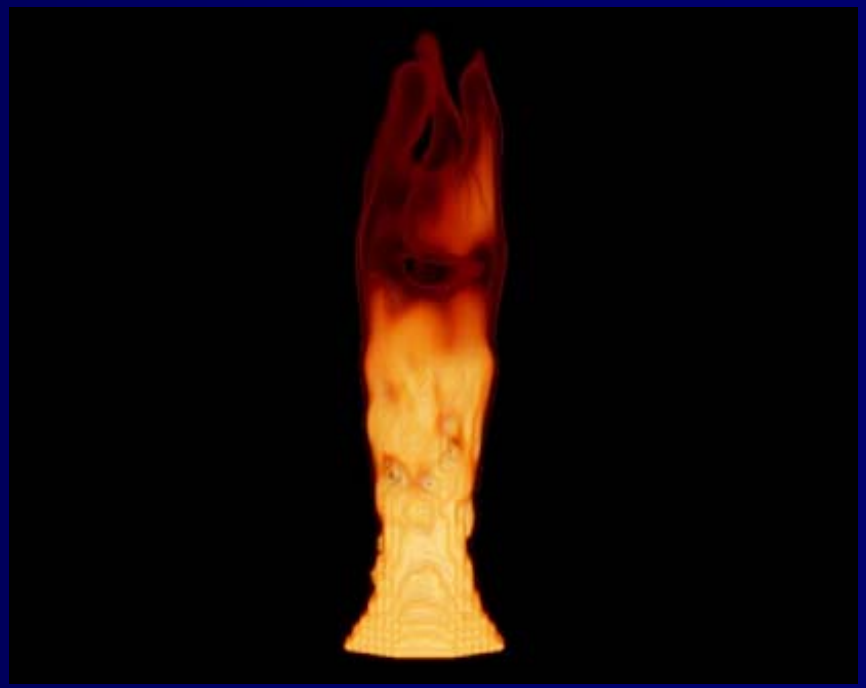
Equilibrium + Correlation



PSRLDM + Lindstedt

1m Heptane Pool Fire
Soot Volume Fraction

Equilibrium + Correlation



PSRLDM + Lindstedt

Acknowledgments

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