Progress on the modeling of multiphase and multimode combustion

Hao Wu, Jeff Labahn, Peter C. Ma, Qing Wang, Matthias Ihme
Multiphase and Multimode Combustion

Referee-Rig Combustor (NJFCP)

Spray & Atomization

Droplet
Evaporation & Combustion

Multimode Combustion

Non-Premixed
Premixed
Mixed Regimes
Multimode Combustion

MODEL ADAPTATION
Adaptive Modeling of Multimode Combustion

Pareto Efficient Combustion Modeling Framework (PEC)

Flamelet-type Models
- Regime-specific
- Computationally efficient

Finite Rate Chemistry
- Regime-agnostic
- Computationally expensive
  - Many species
  - Small time scales

Objective
- Use flamelet models when appropriate
- Use detailed kinetics when necessary
- Achieve good efficiency-fidelity balance
Pareto Efficient Combustion Modeling (PEC)

Key Features

- Local usage of combustion models
- Adaptive assignment of sub-models
- Error control for quantities of interest

\[
\min_{M : \Omega \rightarrow M} \mathcal{E}(M) + \lambda \mathcal{C}(M)
\]

Computational Challenges

- Stiff chemistry
- Load imbalance
  - Model adaptation
  - Clustering of chemical reactivity
Efficient Time Stepping with Stiff Chemistry

- Simpler balanced splitting
  - Separate reaction from advection-diffusion
  - 2-nd order accurate
  - Steady-state preserving
  - Better stability and efficiency
Efficient Time Stepping with Stiff Chemistry

- Semi-implicit integrator (ROK4E)
  - Rosenbrock-Krylov method
  - Explicit-like cost
  - Non-iterative

\[ \text{CPU Time (sec)} \]

\[ 10^{-1} \quad 10^{0} \quad 10^{1} \quad 10^{2} \quad 10^{3} \]

\[ 10^{-8} \quad 10^{-7} \quad 10^{-6} \quad 10^{-5} \quad 10^{-4} \]

Relative error ~ 1.0E-4

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Efficient Time Stepping with Stiff Chemistry

- Dynamic load rebalance
  - 3D DME/air temporal jet simulation

[Images: DME TEMPORAL JET and ODE TIME STEPS]
Efficient Time Stepping with Stiff Chemistry

- Dynamic load rebalance
  - 3D DME/air temporal jet simulation
  - Increased load imbalance with higher CPU count
Efficient Time Stepping with Stiff Chemistry

- Dynamic load rebalance
  - Alleviate scalability issue due to reactivity clustering
  - Redistribute reaction calculation among CPUs

![Graph showing scalability of reaction calculation](chart.png)

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Piloted turbulent partially-premixed DME jet flame

DME Flame-D

- Experimental Configuration
  - Piloted partially-premixed jet flame
  - Re = 29,300
- Numerical Configuration
  - 10 million control volumes
  - 18-species reduced mechanism
  - Combustion models
    - Flamelet/progress-variable (FPV)
    - Finite-rate chemistry (FRC)
    - Adaptive model (PEC)
  - Dynamic thickened flame model

Piloted turbulent partially-premixed DME jet flame

Results

PEC-64 ($\lambda = 0.64$, FPV)
PEC-8  ($\lambda = 0.08$, FPV / FRC)
PEC-0  ($\lambda = 0.00$, FRC)

\[ \min_{\mathcal{M} : \Omega \rightarrow M} \mathcal{E}(\mathcal{M}) + \lambda \mathcal{C}(\mathcal{M}) \]
Piloted turbulent partially-premixed DME jet flame

Results

![Graphs showing temperature and CO concentration profiles at different x/D values (x/D = 5, x/D = 10, x/D = 20).](image)

PEC-8

![Imagery and data visualization for PEC-8, including spatial distribution of Z_p, T, and X_CO.](image)
Piloted turbulent partially-premixed DME jet flame

Results

![Graphs showing X_CO and FRC Usage % vs. lambda for x/D = 10 and 20.](image)

![Graphs showing normalized cost vs. lambda for x/D = 10 and 20.](image)
Summary

- Combustion model adaptation (PEC)
  - Combined usage of flamelet-type and finite rate chemistry models
  - Adaptive model assignment with error control
  - Efficient and scalable time stepping for finite rate chemistry
  - LES-PEC simulations of DME flame-D
    - Improved prediction of CO emission
    - 2X reduction in cost

Related publications:

