A Flamelet Generated Manifold Model for Partially Premixed Laminar Flames

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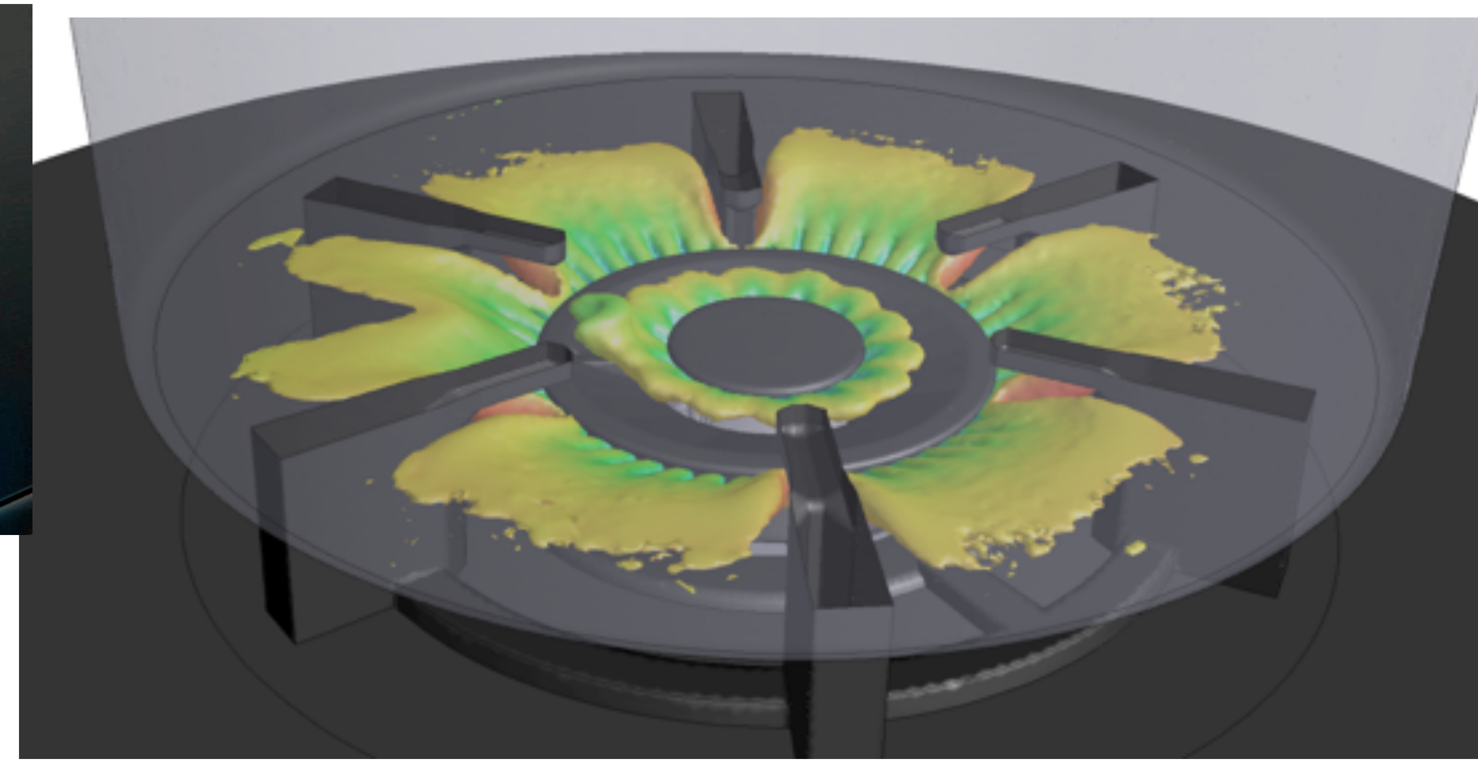
Why: partially premixed flames in stove burners

- Computational design of stove-top burners:
  - Heat-transfer efficiency
  - Pollutants: NOx, CO
  - Operational safety, certification (liftoff, flashback)

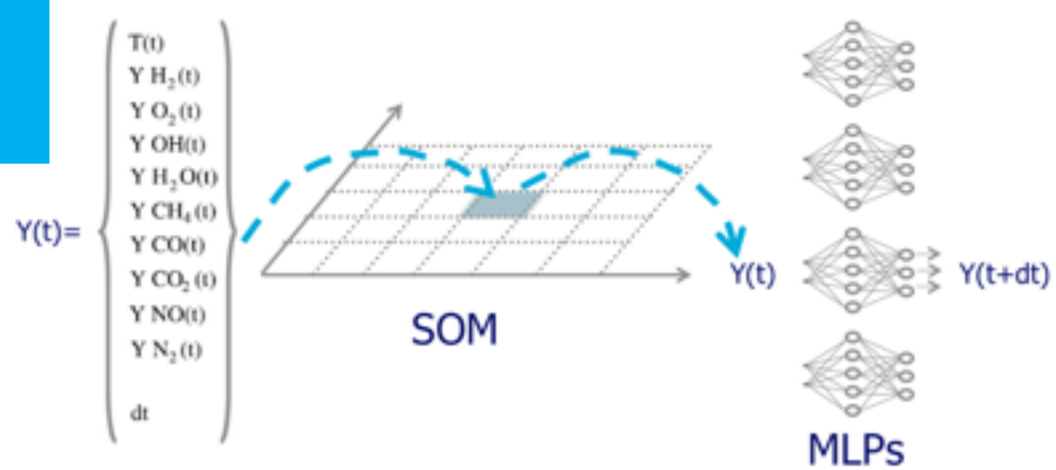


- Computations are expensive:
  - Tens to hundreds of species
  - Transport-equation system is stiff: wide range of timescales
- “Reduced” chemical systems are an alternative…
    - But still expensive and not available for all fuels (eg propane, butane)

Route to more economical calculations

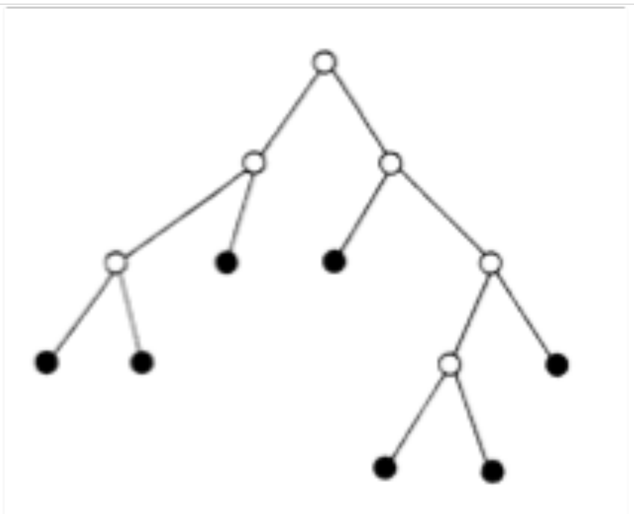
- Among other possibilities…

Artificial Neural Networks



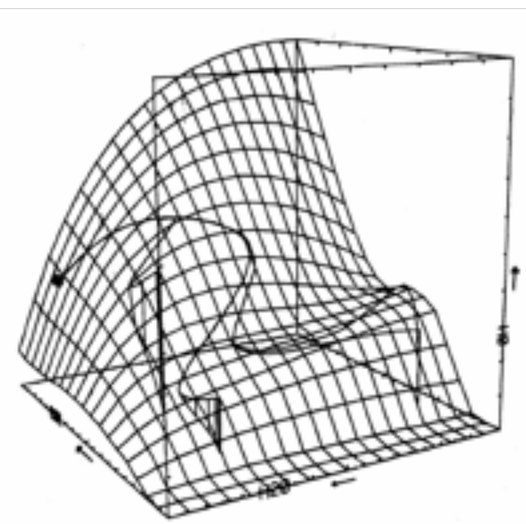
J. Blasco, N. Fueyo, C. Dopazo, and J. Ballester. Modelling the temporal evolution of a reduced combustion chemical system with an artificial neural network. Combustion and Flame, 113(1–2):38 – 52, 1998.

In Situ Adaptive Tabulation



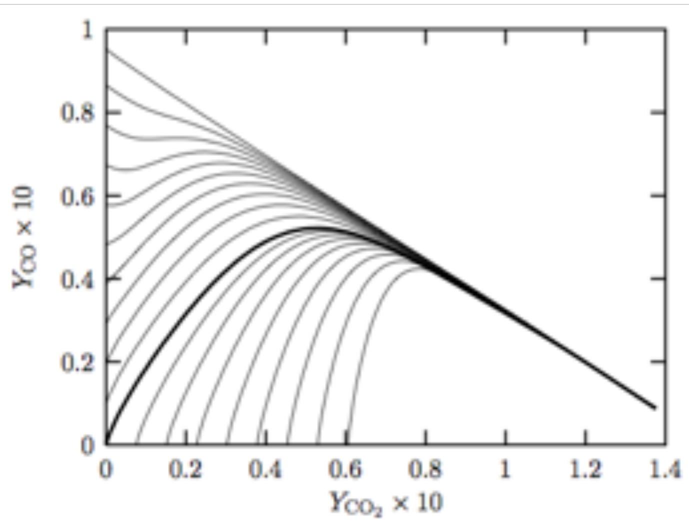
S. B. Pope. Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation. Combustion Theory and Modelling, 1(1):41–63, 1997.

Intrinsic Low Dimensional Manifolds



U. Maas and S. Pope. Simplifying chemical kinetics: Intrinsic low-dimensional manifolds in composition space. Combustion and Flame, 88(3–4):239 – 264, 1992.

Flamelet Generated Manifolds



J. van Oijen, F. Lammers, and L. de Goey. Modeling of complex premixed burner systems by using flamelet-generated manifolds. Combustion and Flame, 127(3):2124 – 2134, 2001.

Two approaches in this presentation

burnerFOAM

- DI: Direct integration of the thermochemistry
  - Integrates all the equations for all the species, inc chemical reaction
  - Typically 16 to 50 scalars (species)
  - Accurate (?) but expensive

fgmFOAM

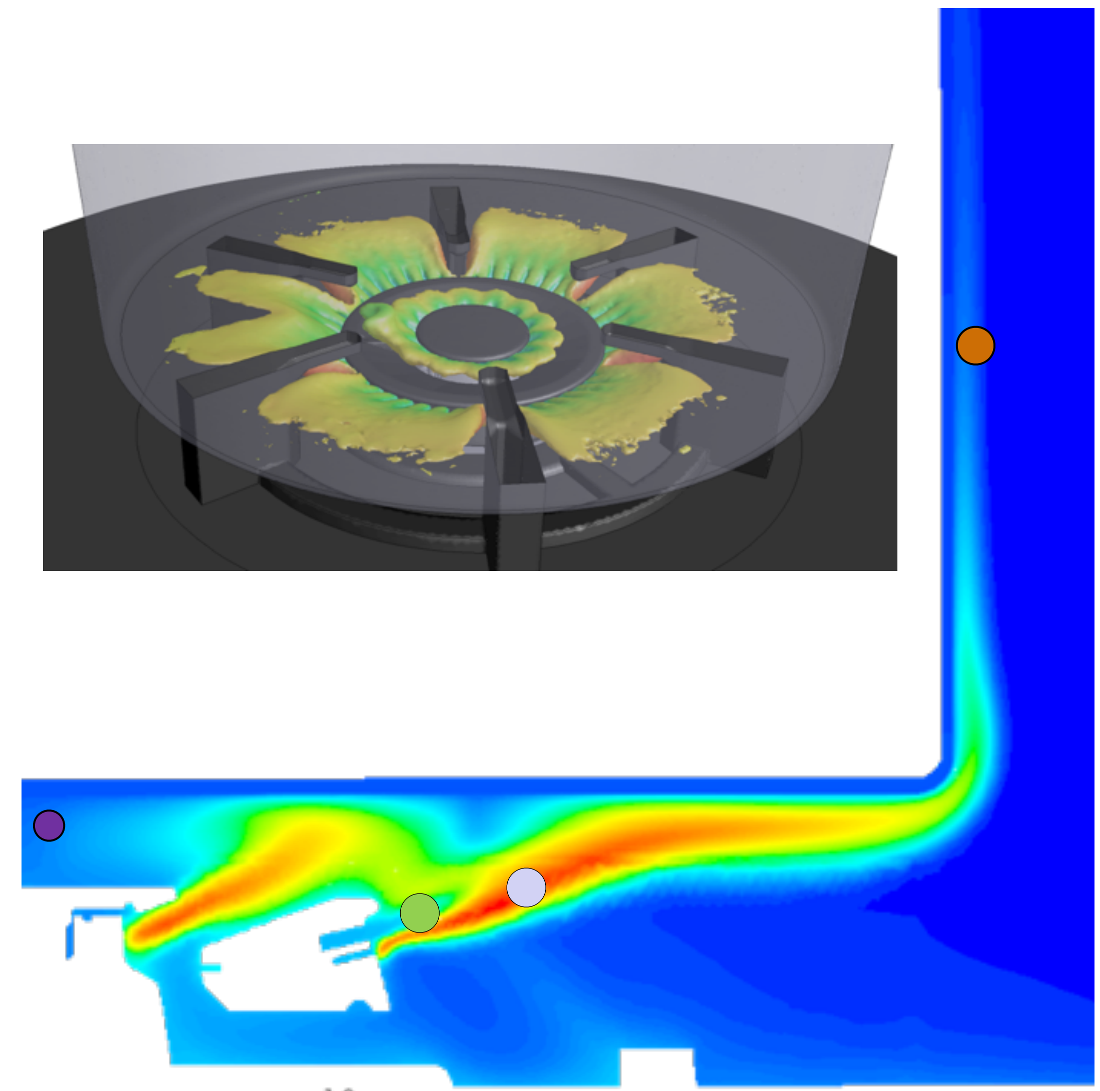
- FGM: Pre-calculation and storage of a reduced system
  - Explores, ex-ante, the compositional space, and tabulates a reduced chemistry
  - Typically 3 scalars define the thermochemistry (“controlling variables”, “FGM coordinates”)
  - Cheap but less accurate

FGM generation

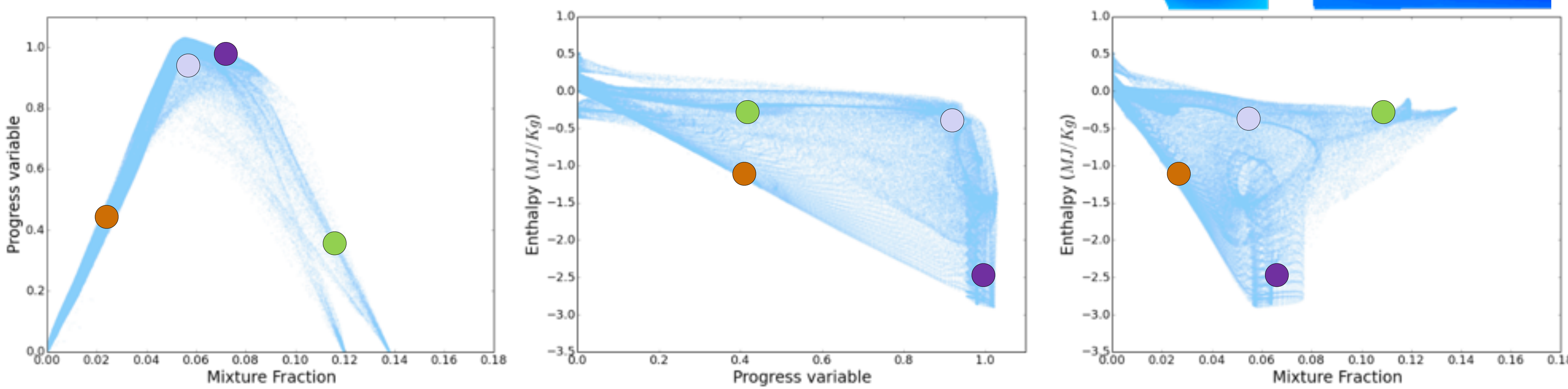
The challenge of accessing the thermochemical space

Thermochemical space accessed in a simulation

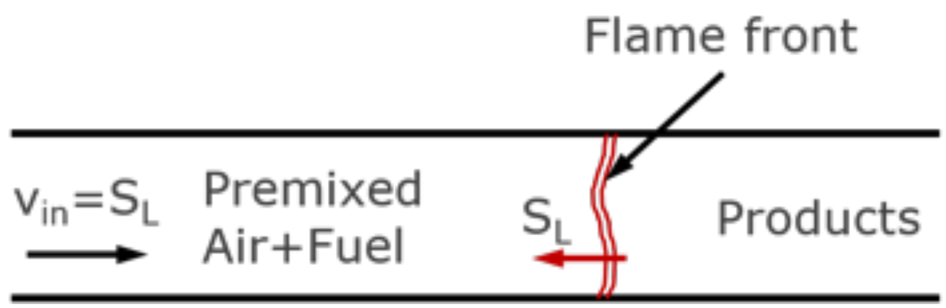
- Scatter plot of thermochemical space with direct integration of chemistry
- Projected on selected planes of compositional space
- Four selected points in physical space

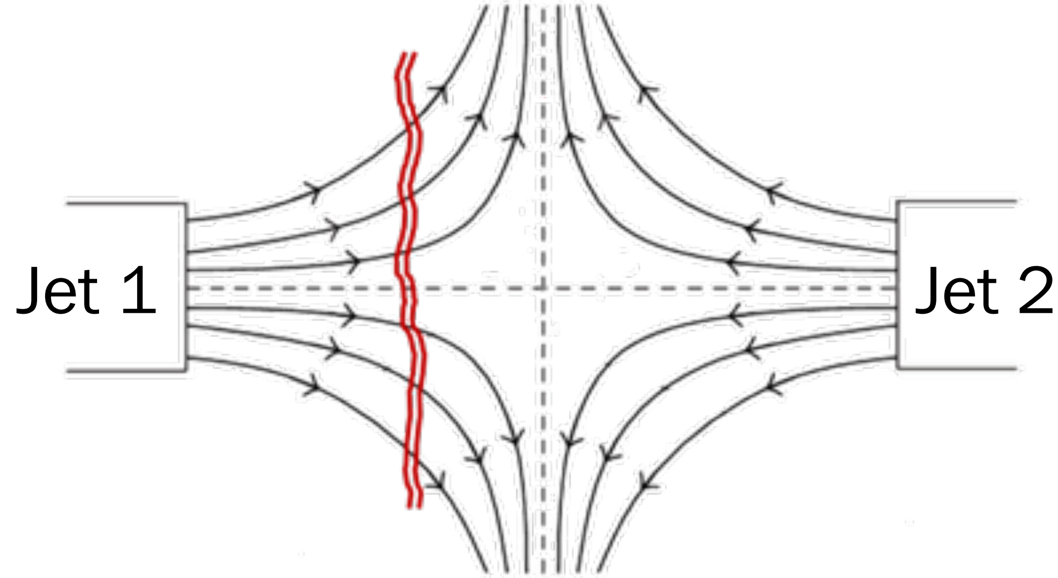


Direct integration (burnerFOAM)



Compositional space exploration strategies



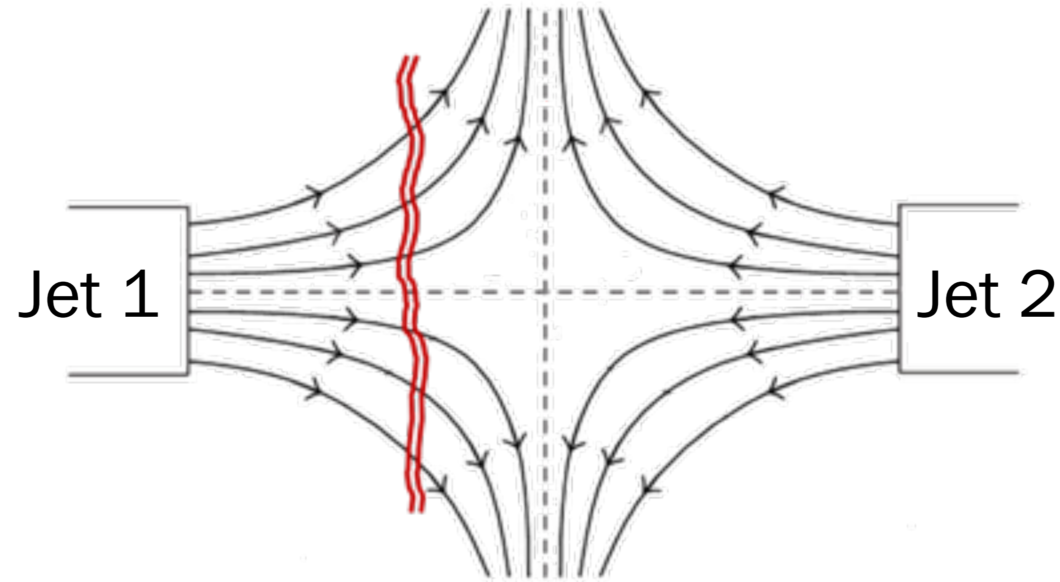


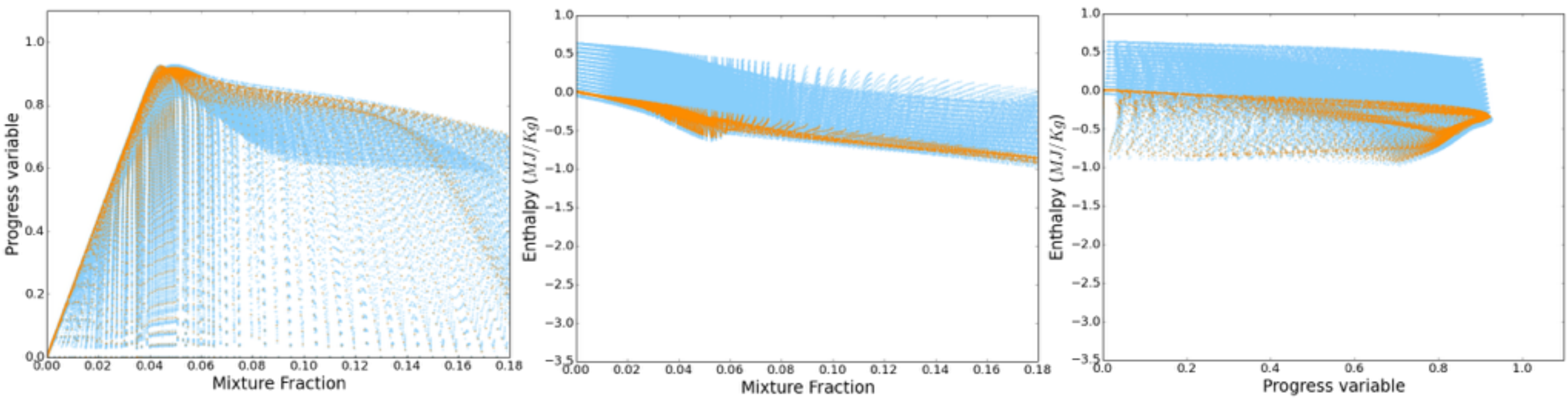
- Free premixed flames
  - Adiabatic, or moderate heat extraction
  - Composition must be within flammability limits
  - Weak effect of differential diffusion

- Opposed-jet flames
  - Rich-lean jets, air-lean, adiabatic
  - Air-premixed jets, heat extraction

Adiabatic “family”

- Rich-lean, opposed jet flames
- Several inlet temps (orange: one set of temps for illustration)
- No heat extraction





“Low-enthalpy” families

- Opposed-jet flames, with several inlet compositions; heat extraction

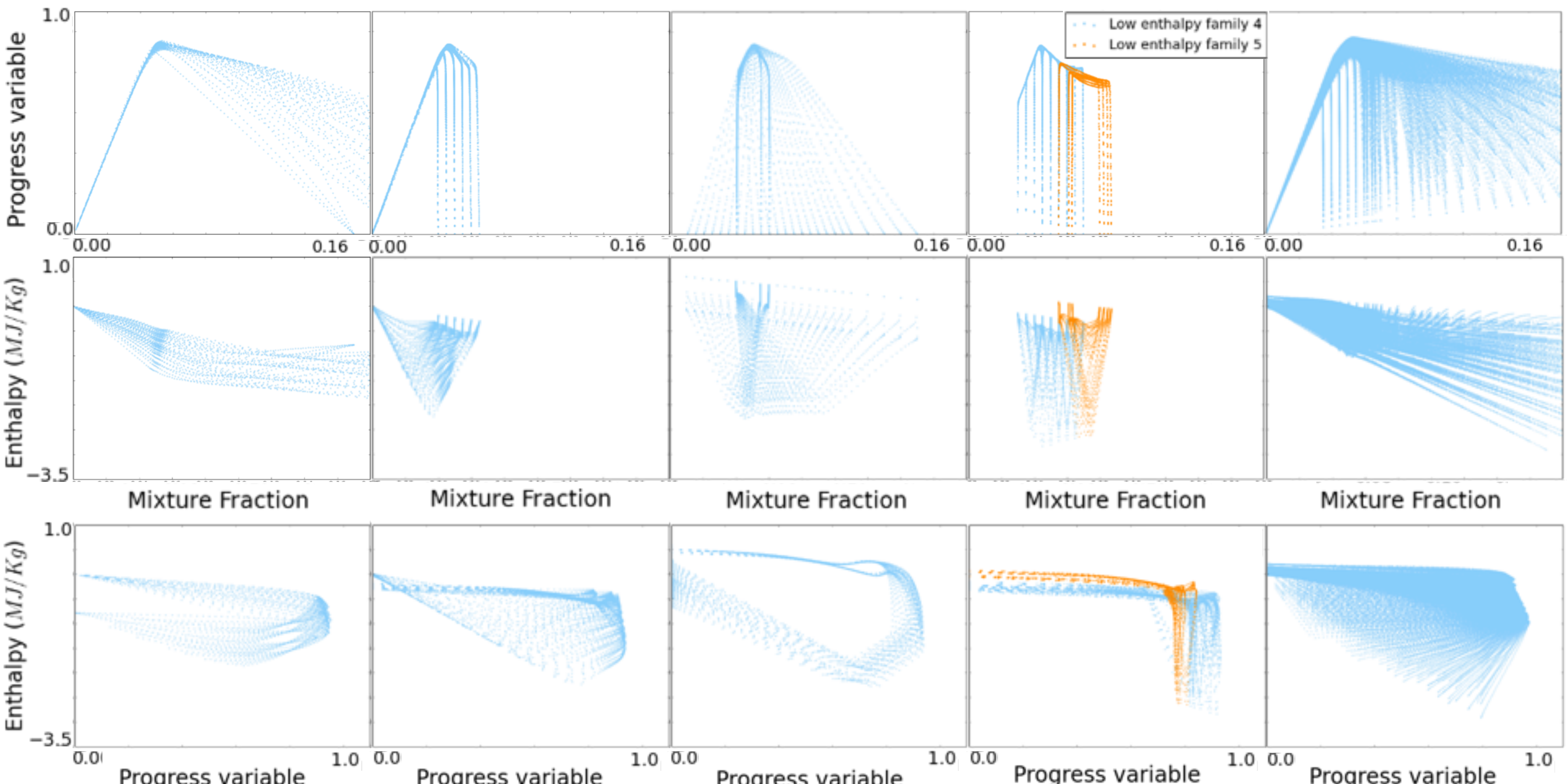
1
- Air 300K><premixed 300K
- Heat extraction along whole domain

3
- Air 300K>< various around stoic 300K
- Heat extraction along lean side

2
- Stoichiometric 900K>< various premixed 300K
- Heat extraction along one side to fix temp

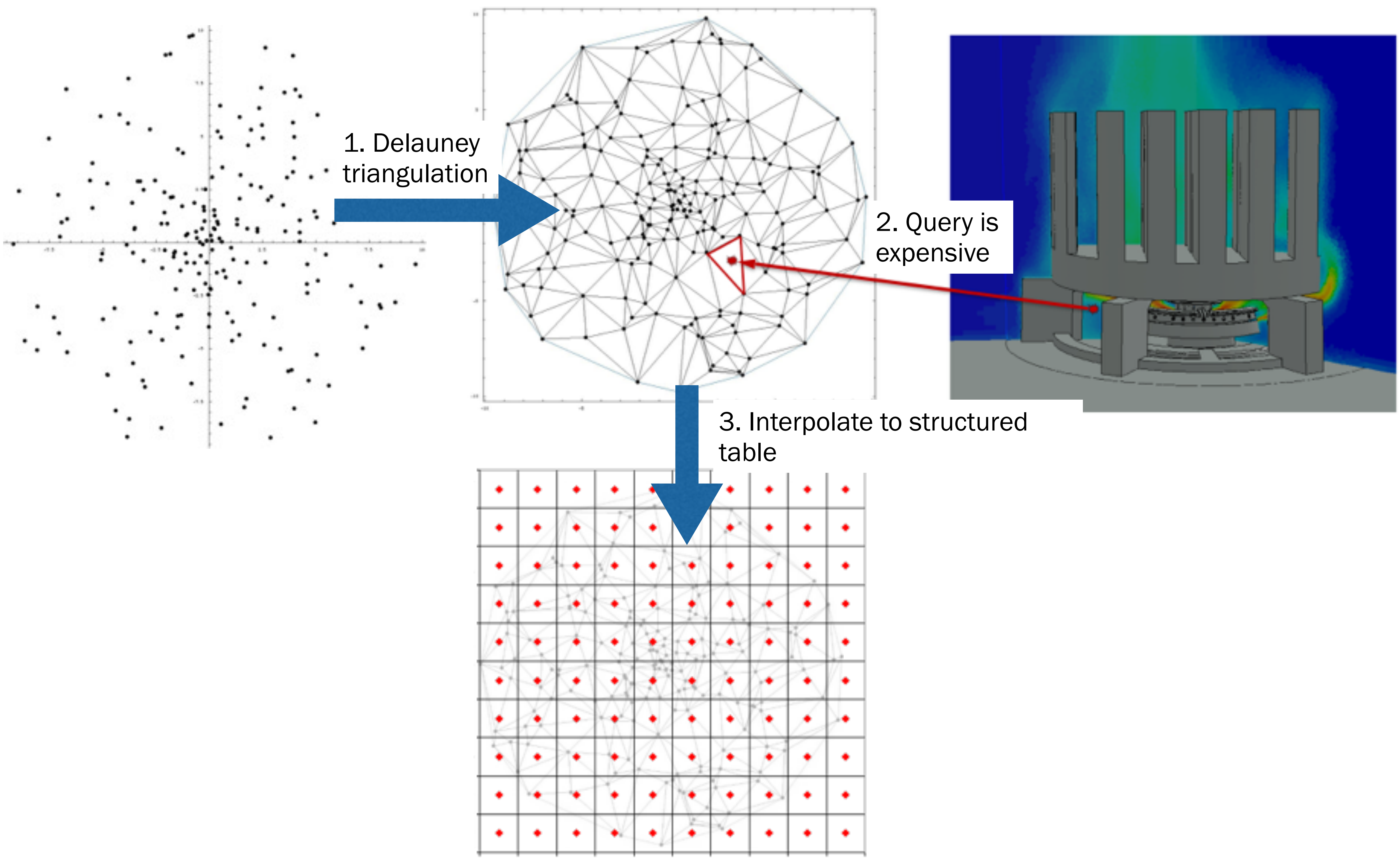
4, 5
- Premixed 300K>< ditto
- Ditto 600K Heat extraction in a region

6
- Cold (300K), partly burnt mixtures in both jets

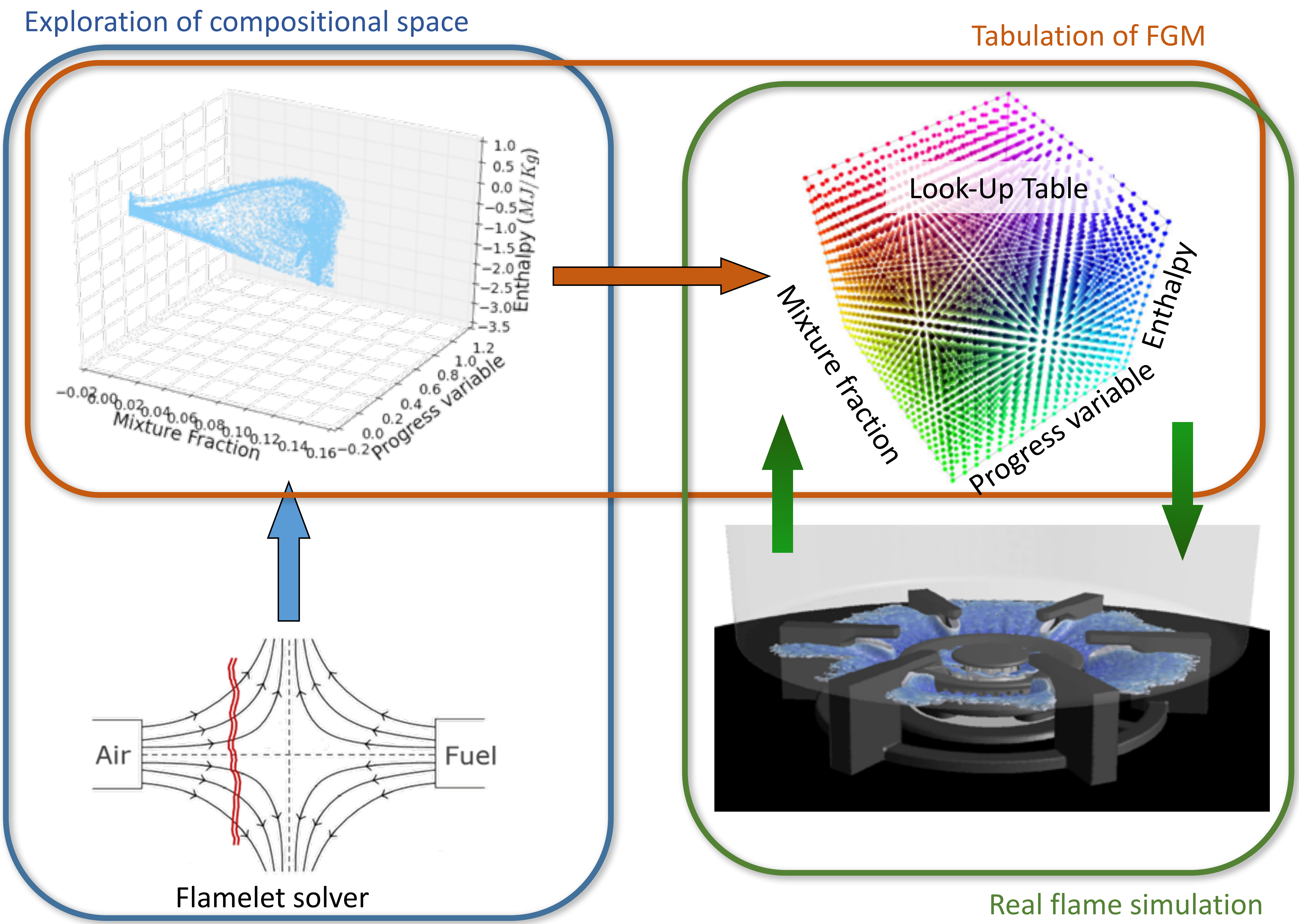


Storage of the thermochemical space

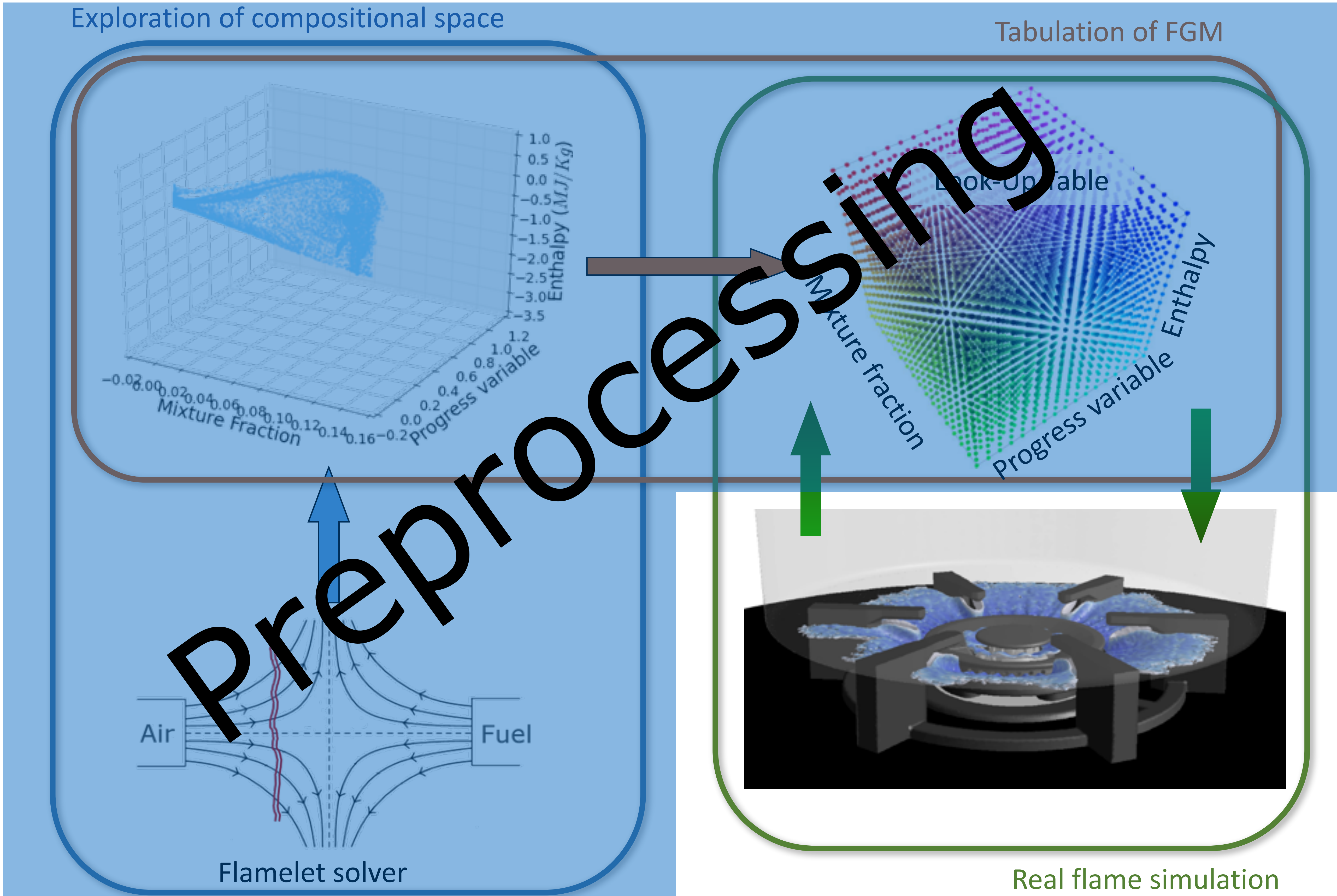
- Delauney triangulation to structured table



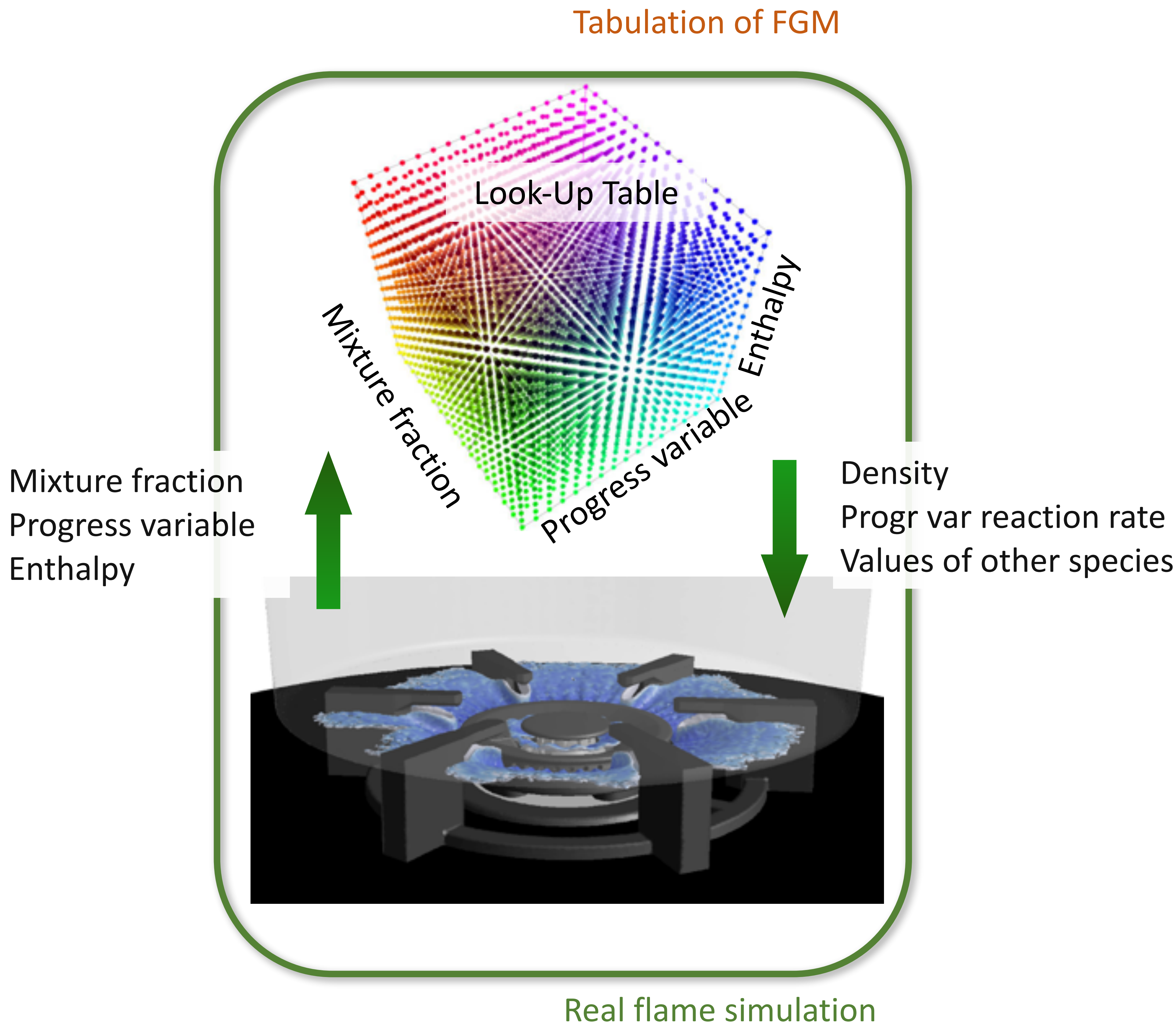
FGM usage overview



FGM usage overview



FGM usage overview



Meanwhile, in CFD (fgmFOAM)

- Solve, continuity, momentum, and ecs for three manifold controlling vars
- In a 3D manifold (FGM3d):
  - Mixture fraction (non-reactive)

$$\frac{\partial(\rho Z)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} Z) = \nabla \cdot \left(\frac{k}{C_p} \nabla Z \right)$$

  - Progress variable: linear combination of some reacting species, indicates reaction progress; mostly using H2O and CO2: $\mathcal{Y} = y_{H_2O}/M_{H_2O} + y_{CO_2}/M_{CO_2}$

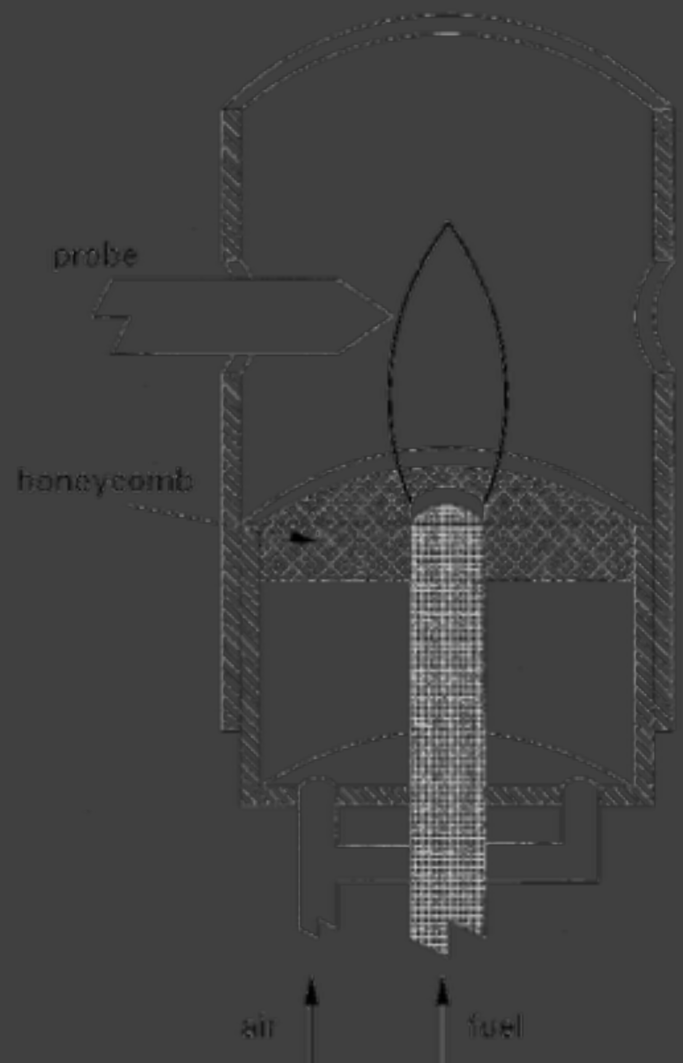
$$\frac{\partial(\rho \mathcal{Y})}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} \mathcal{Y}) = \nabla \cdot \left(\frac{k}{Le_{\mathcal{Y}} C_p} \nabla \mathcal{Y} \right) + S_{\mathcal{Y}}$$

  - Enthalpy

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} h) = \nabla \cdot \left(\frac{k}{C_p} \nabla h \right) + \nabla \cdot \left[\frac{k}{C_p} \sum_{i=1}^{N_s} \left(\frac{1}{Le_i} - 1 \right) h_i \nabla y_i \right] + \dot{q}_r$$

Test on Yale burner

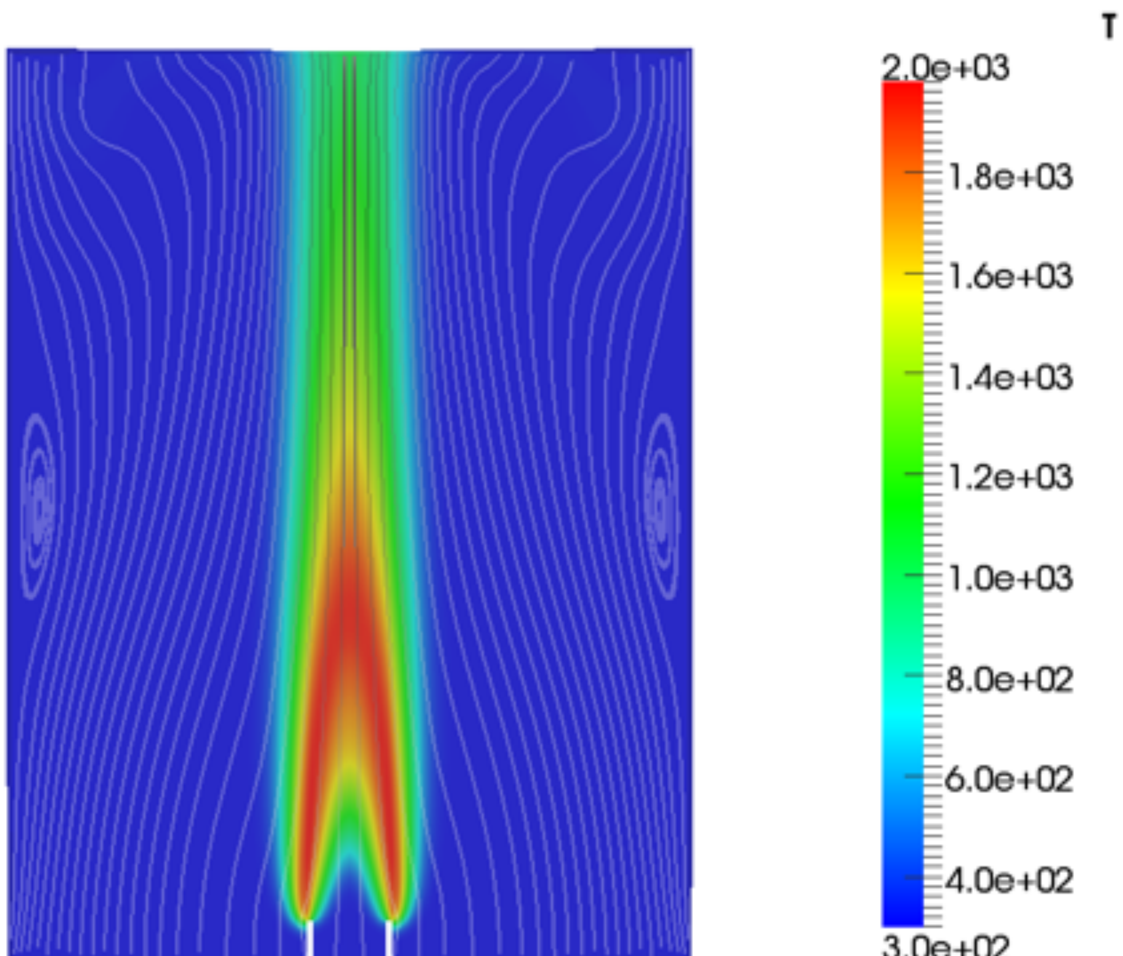
Laboratory burner, simple geometry, experimental data

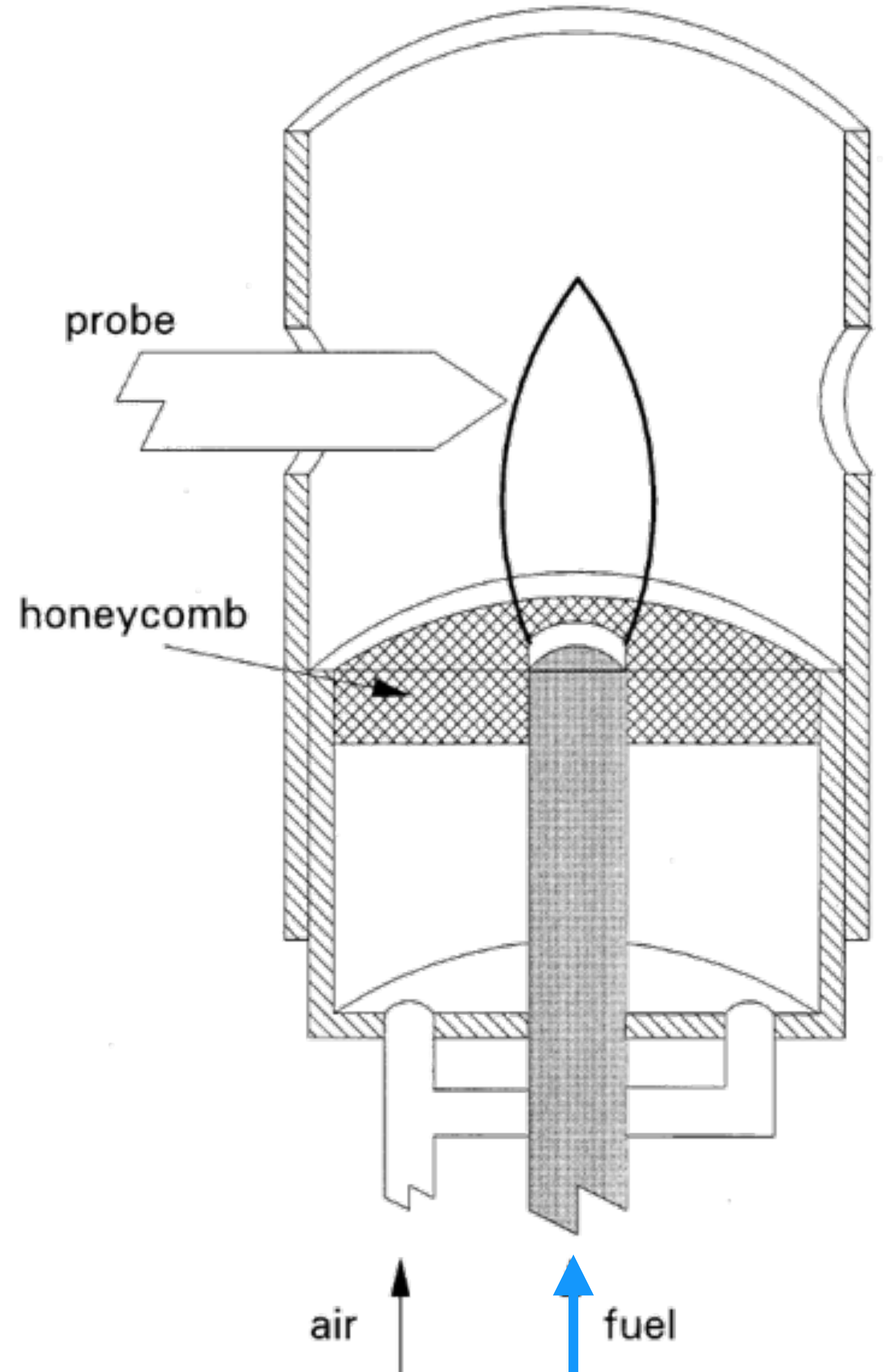


Yale burner

- Yale burner M. Smooke, C. McEnally, L. Pfefferle, R. Hall, and M. Colket. Computational and experimental study of soot formation in a coflow, laminar diffusion flame. Combustion and Flame, 117(1–2):117 – 139, 1999
- Several degrees of premixing

Direct integration (burnerFOAM)

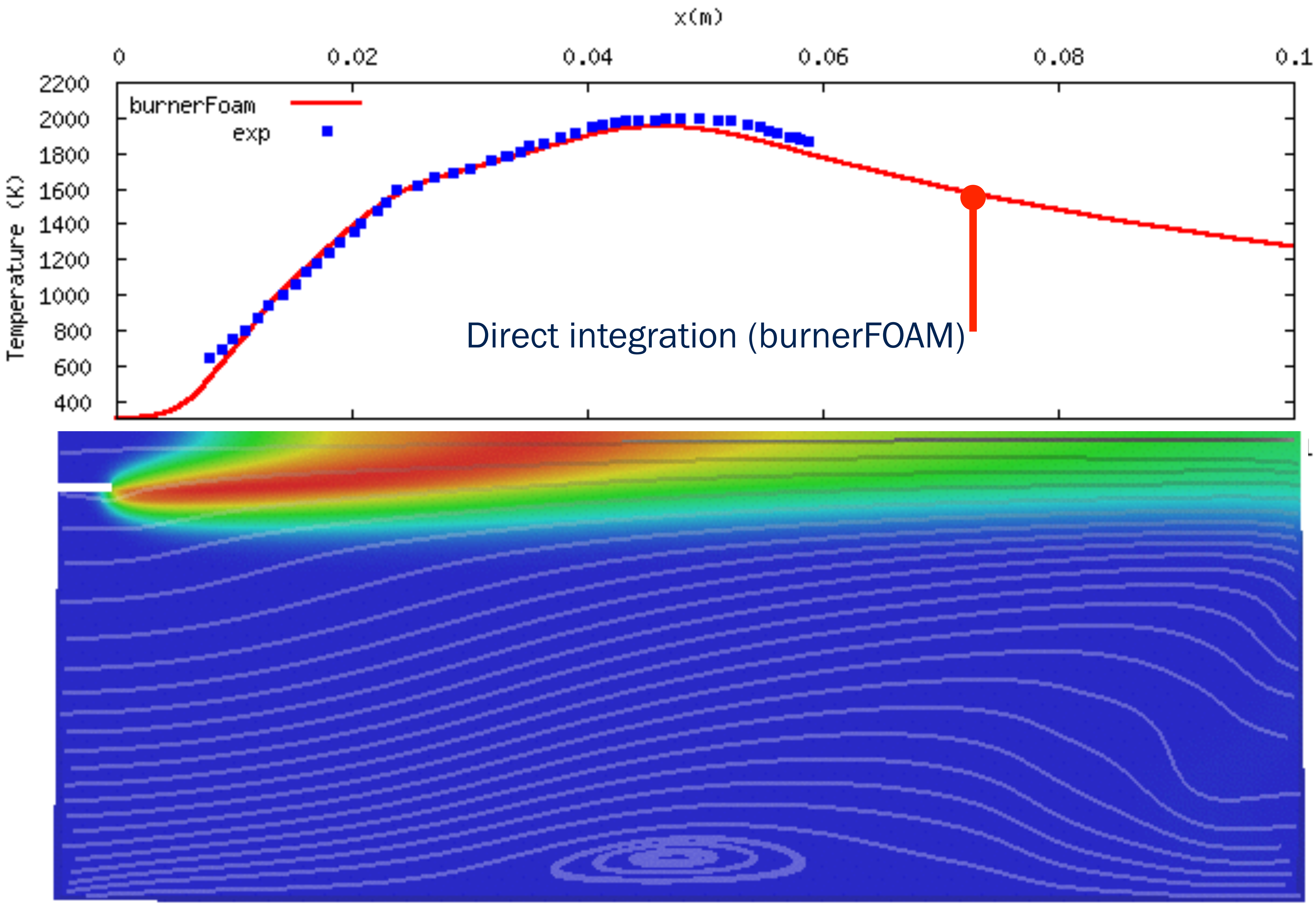




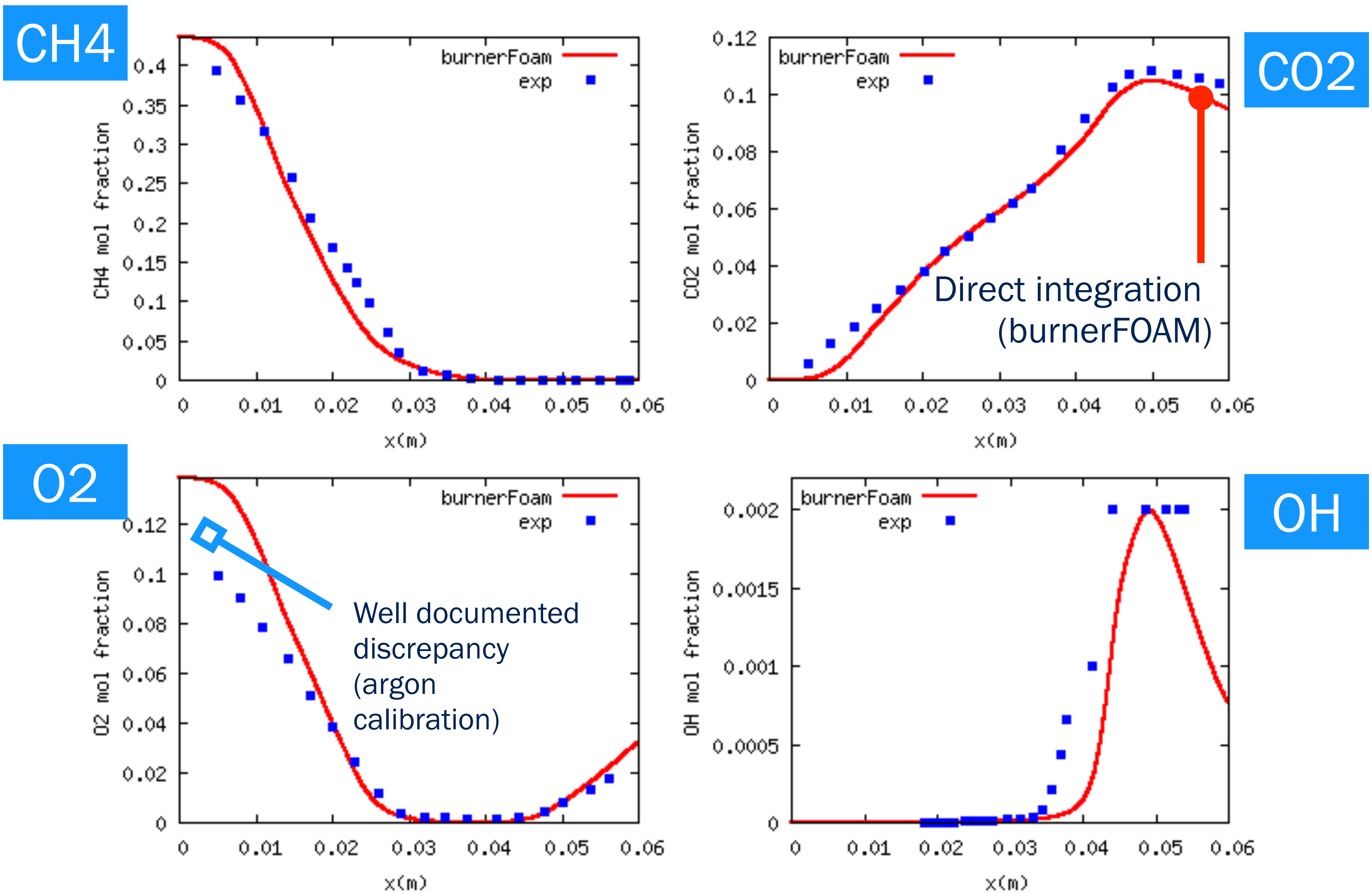
Air-methane premixed primary (ϕ=6.2)

Yale results (burnerFOAM): Temperature

- Direct integration (burnerFOAM): Temperature along axis

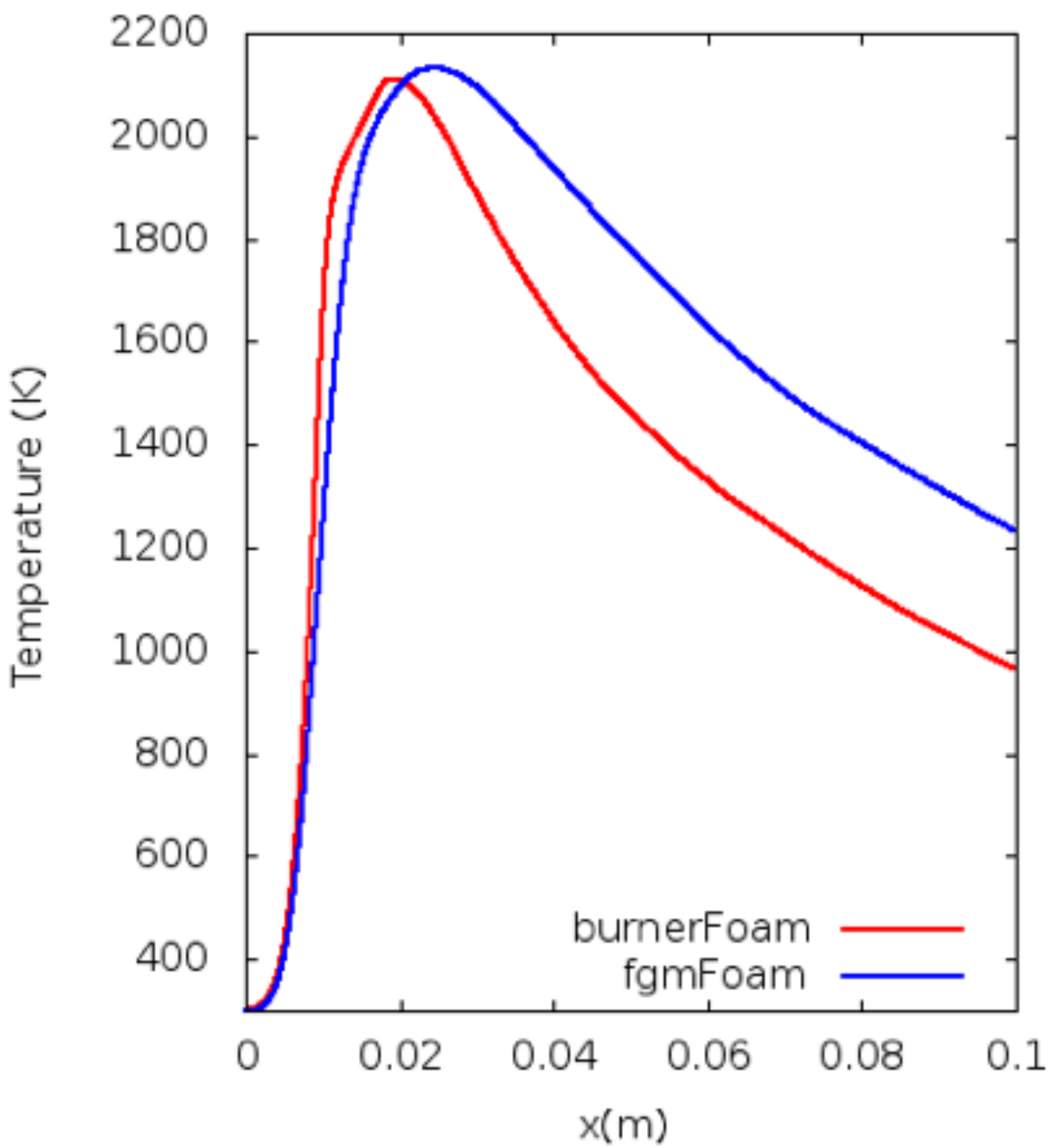


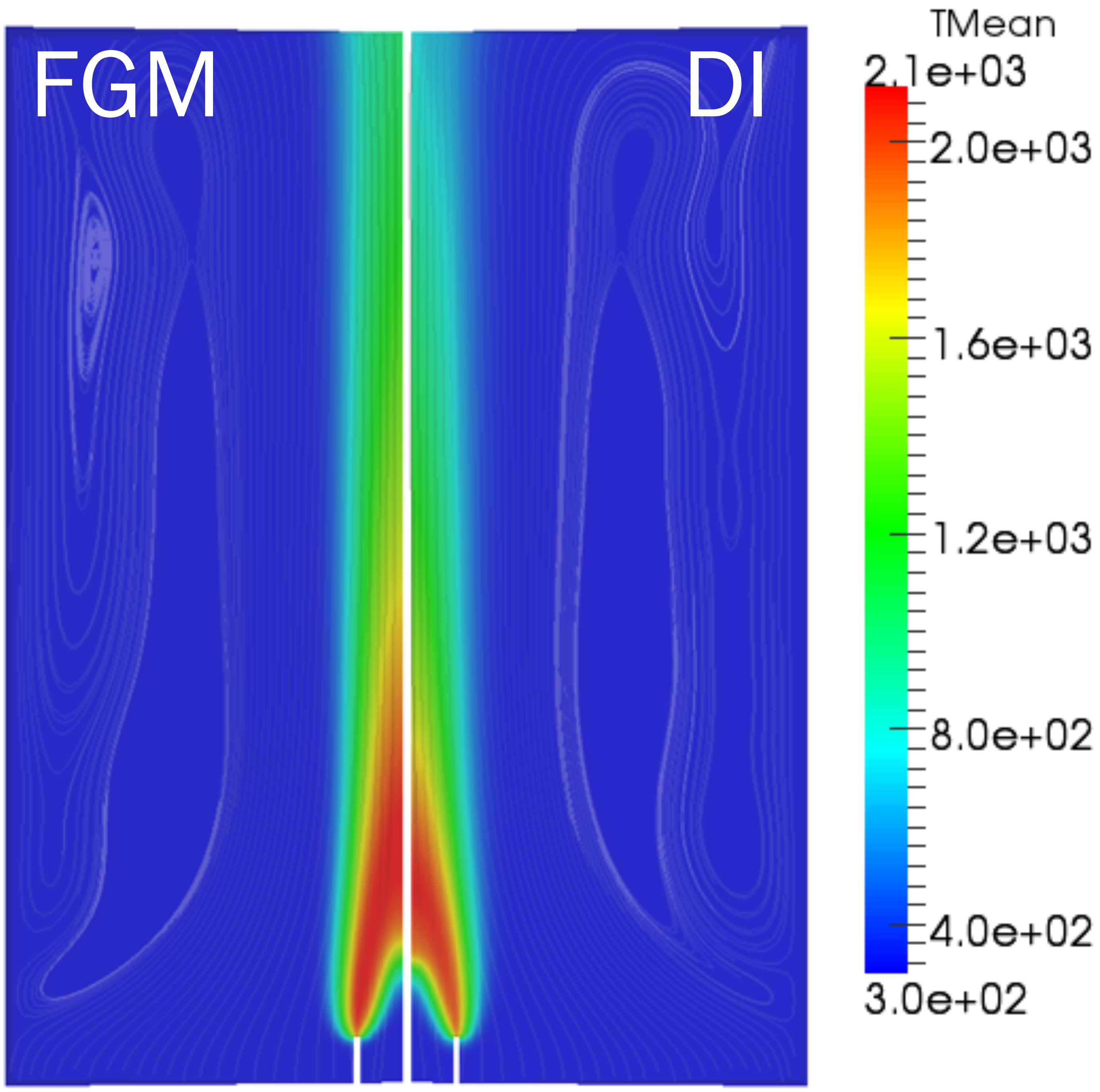
Yale results (burnerFOAM): Species



fgmFOAM vs burnerFOAM (direct integration)

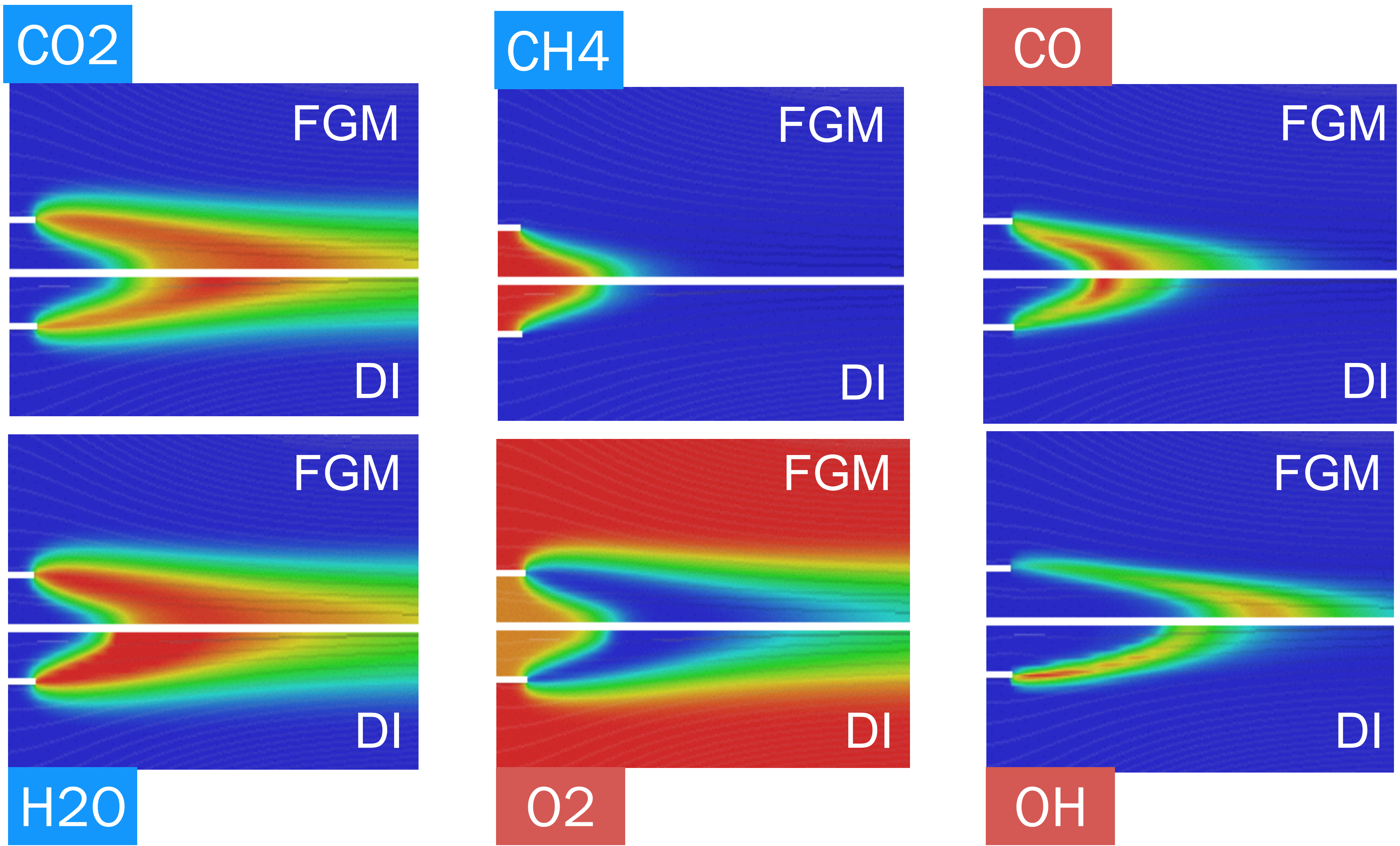
- Smooke (16 species) mechanism in burnerFOAM
- Temperature, K





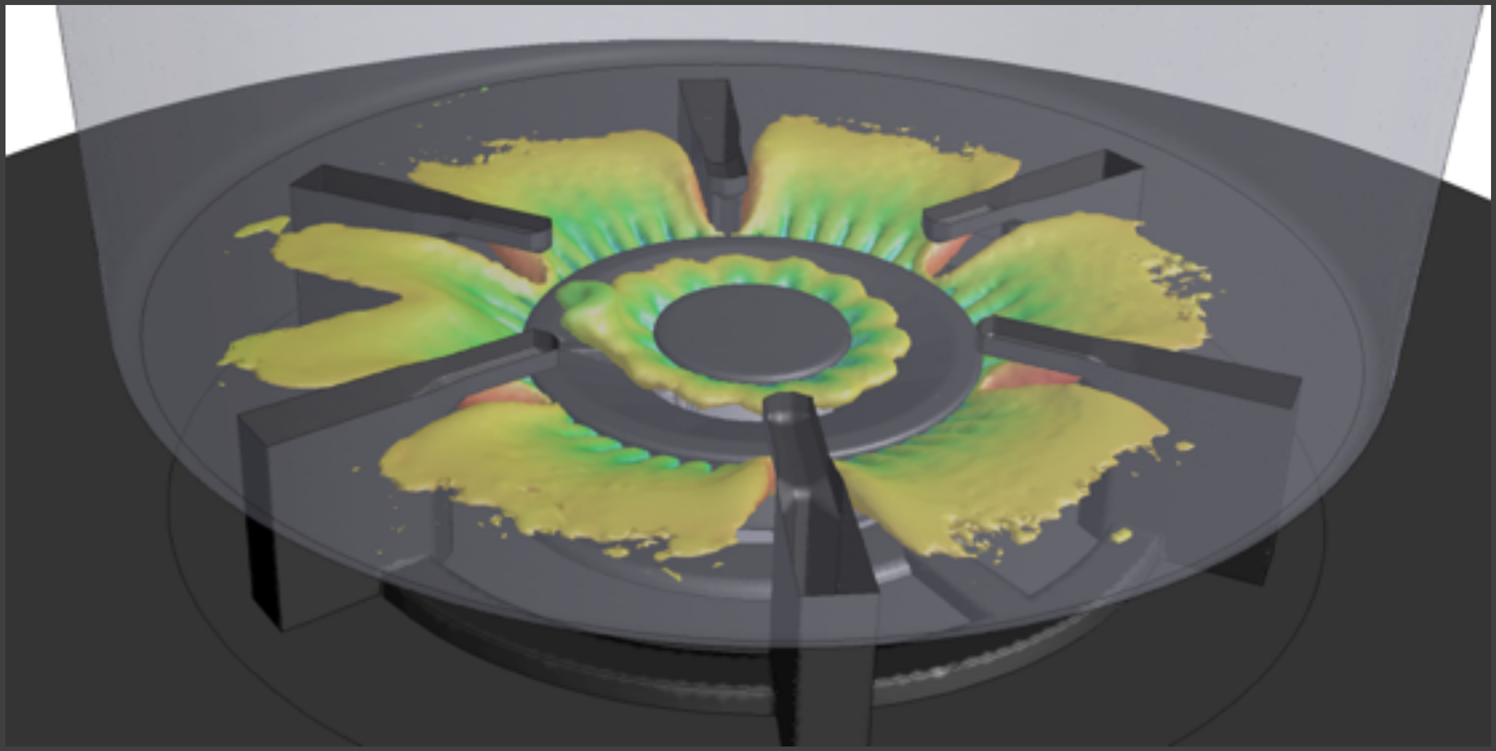
fgmFOAM vs burnerFOAM (direct integration)

- Smooke (16 species) mech in burnerFOAM
- Species. Red label: not transported in FGM



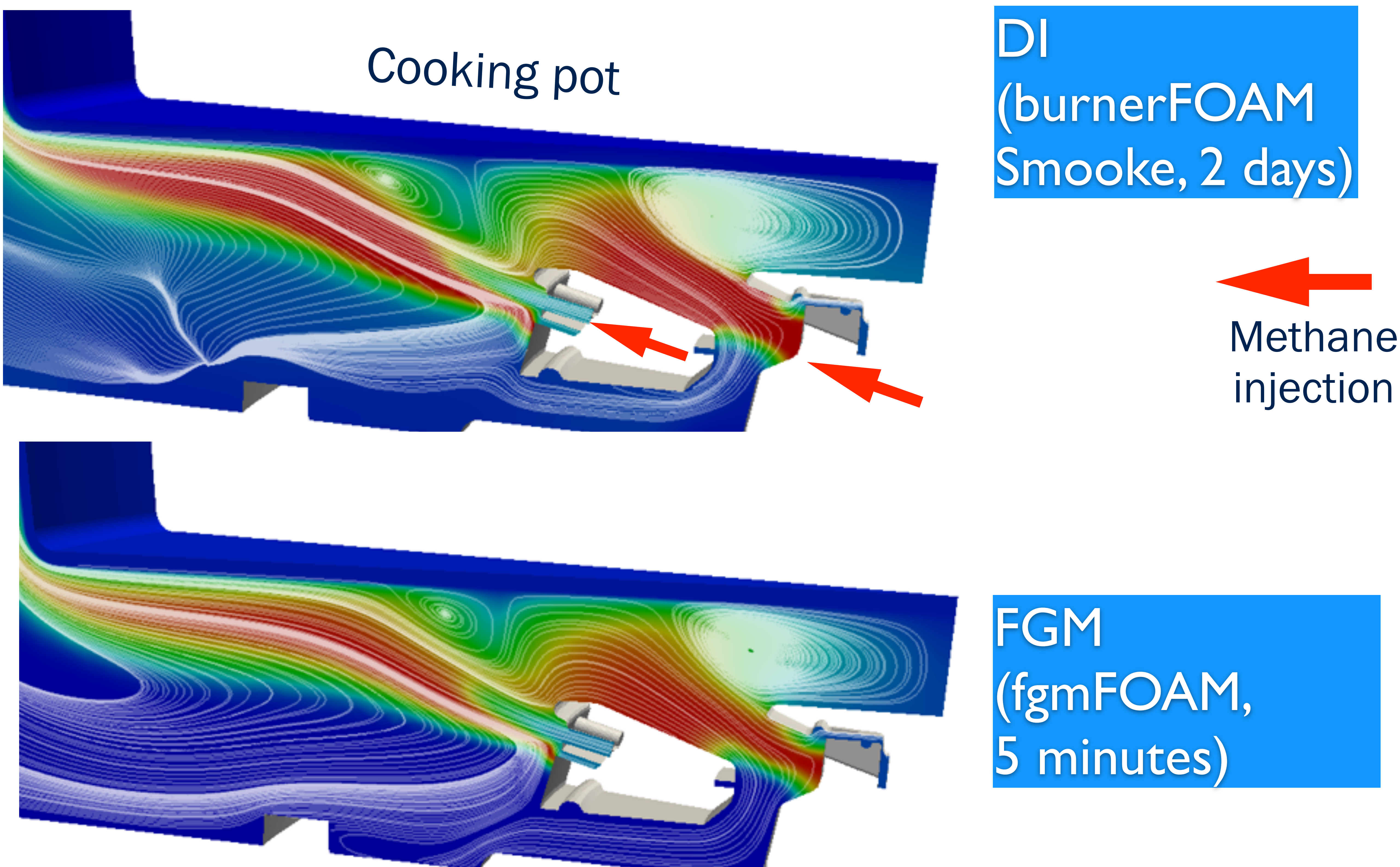
Test on cooking (stove-top) gas burner

Complex geometry, no experimental data



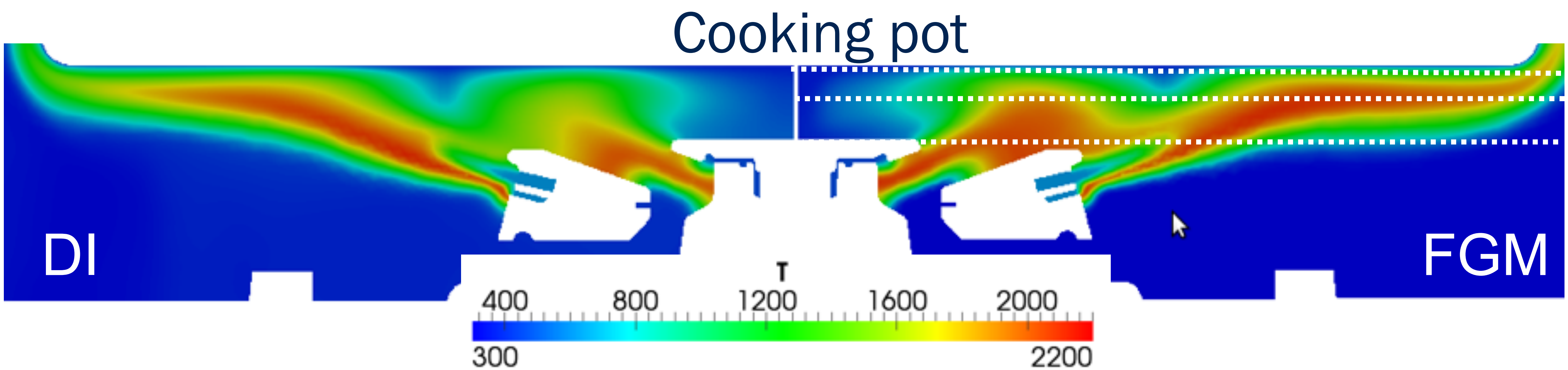
Comparison of instantaneous fields

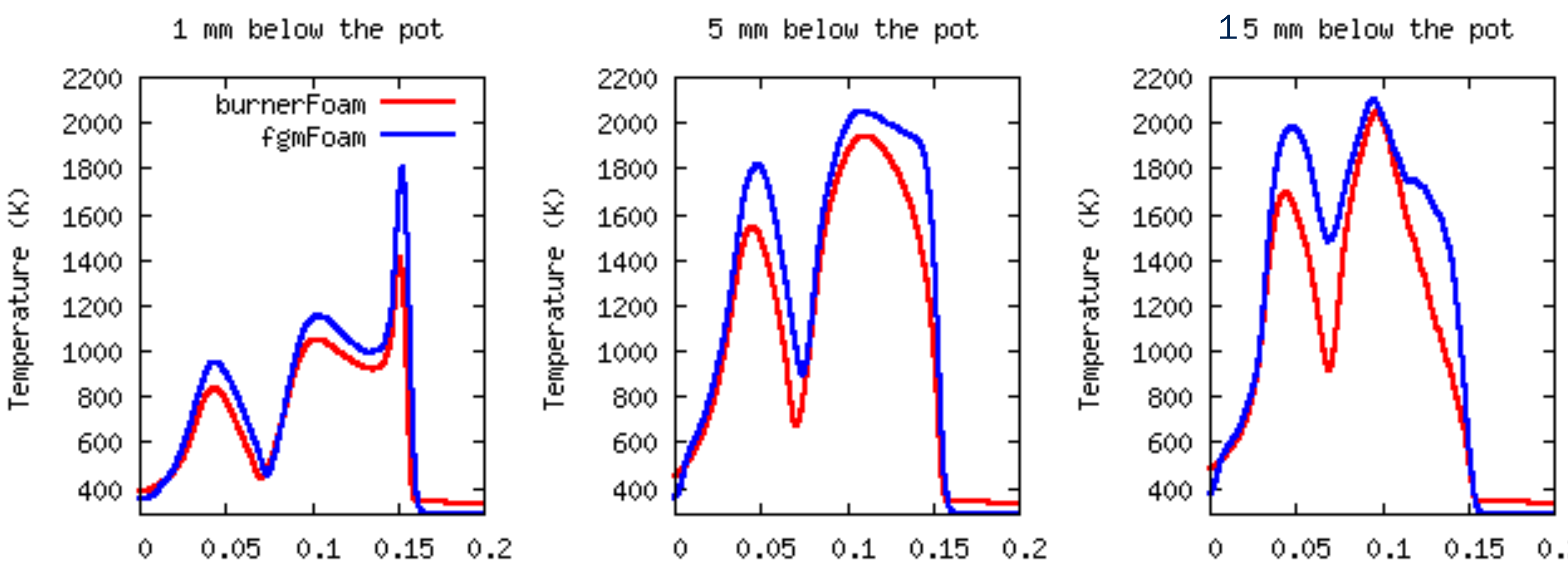
- Temperature and streamlines



Average temperatures (K)

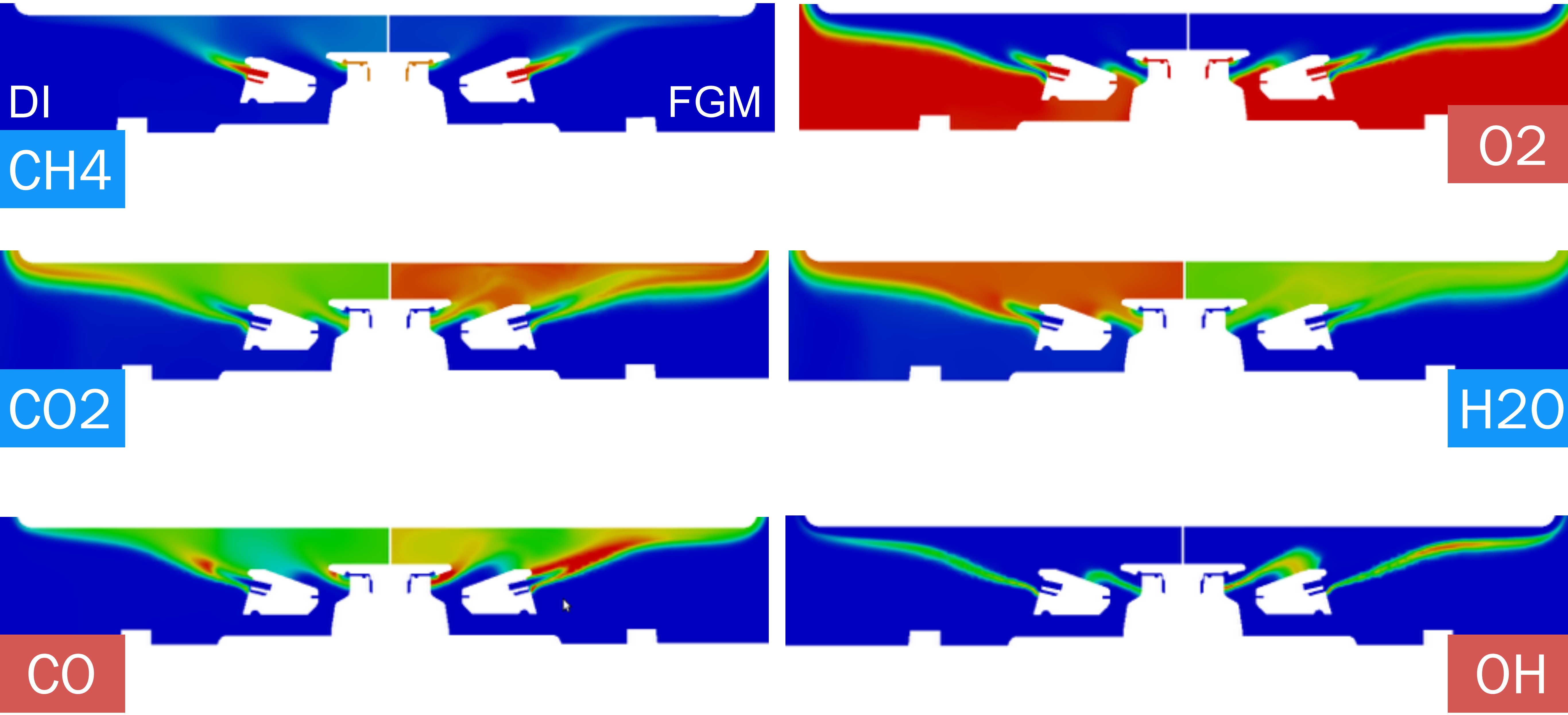
- fgmFOAM vs burnerFOAM (direct integration)





Species

- Red label: not transported in FGM



OpenFOAM implementation

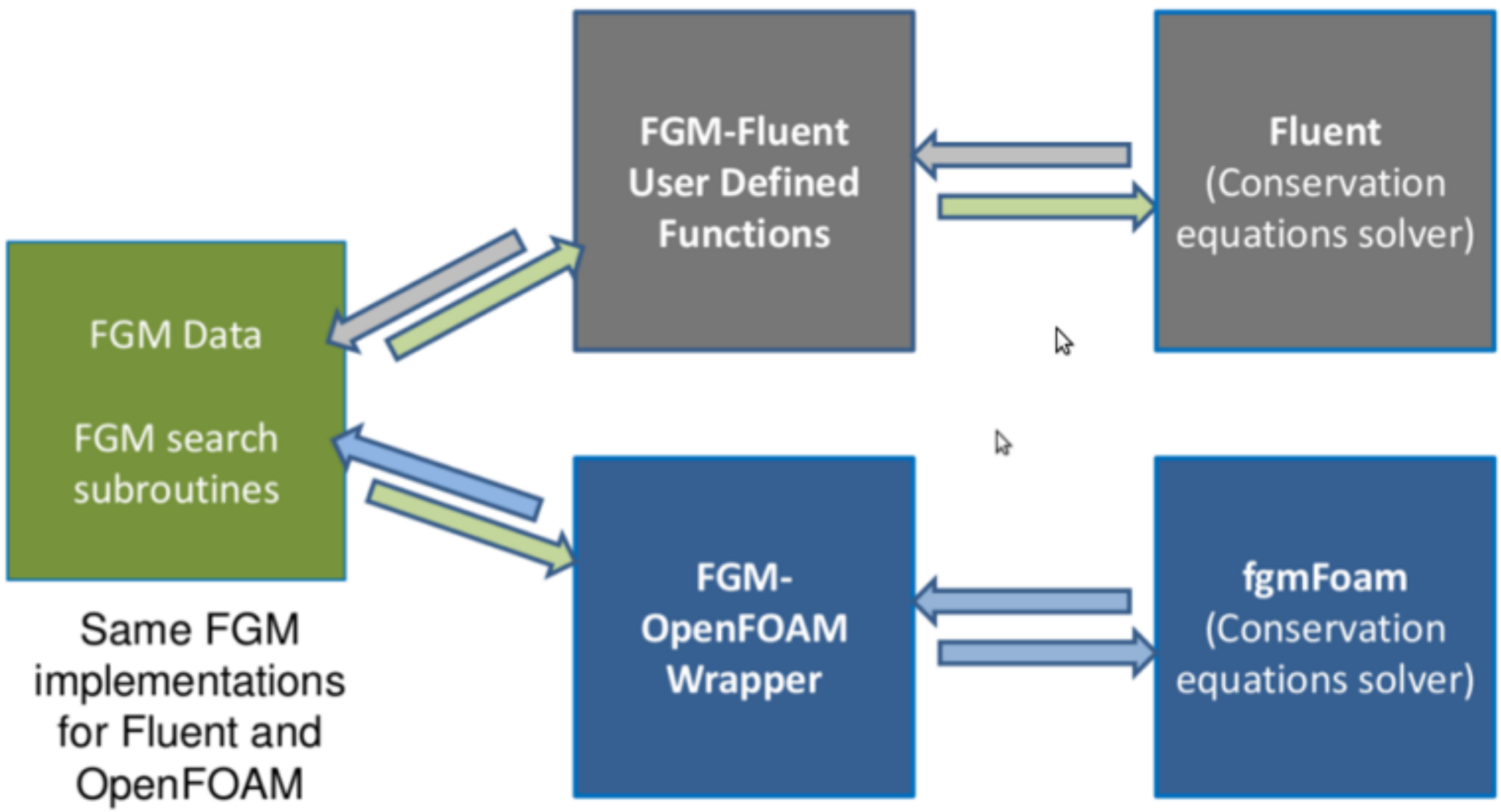
burnerFOAM solver

- Derived from reactingFoam (OF-v2.2.0)
  - Our own mass-transport library
  - Expanded for conjugate heat transfer (solids, P1 radiation)

```
burnerSolver/
├── burnerFoam/
│   └── burnerFoam.C ...................................... main program
│       └── Iterative loop:
│           ├── pEqn.H
│           ├── UEqn.H
│           ├── EEqn.H .................. calls to reaction and radiation modules
│           └── YEqn.H .................. call to MassTransportLibrary for diffusion
├── MassTransportLibrary/
│   ├── diffusivityModels/ .................. binary diffusivity coefficients
│   └── multispeciesTransportModels/ ...... multicomp diffusion-flux;
│                                           & solve equation for species
└── AbsorptionCoeff/ .......................... Radiation coefficients
```

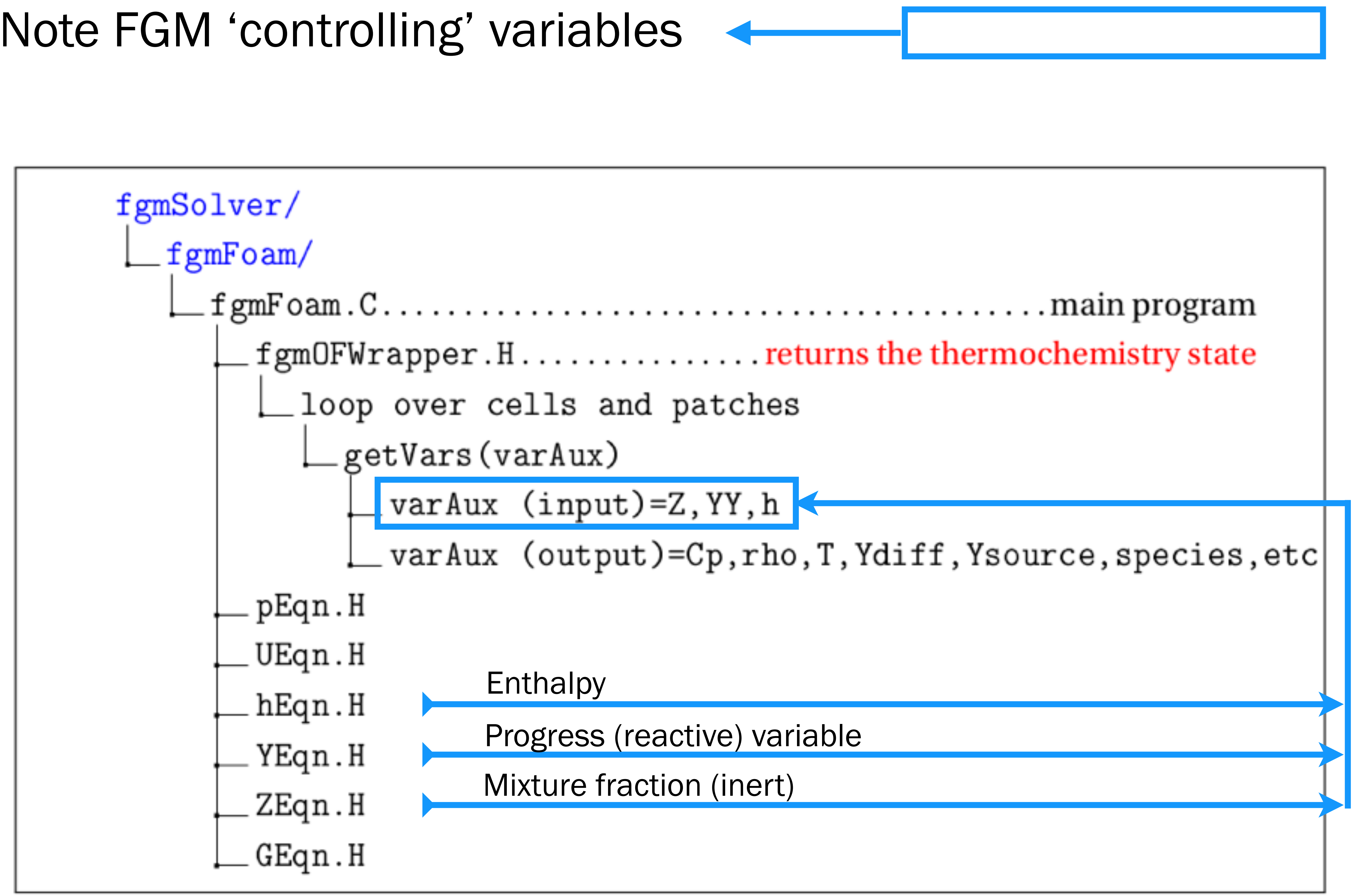
fgmFOAM solver

- Implemented via interface that can be used with OpenFOAM or ANSYS Fluent



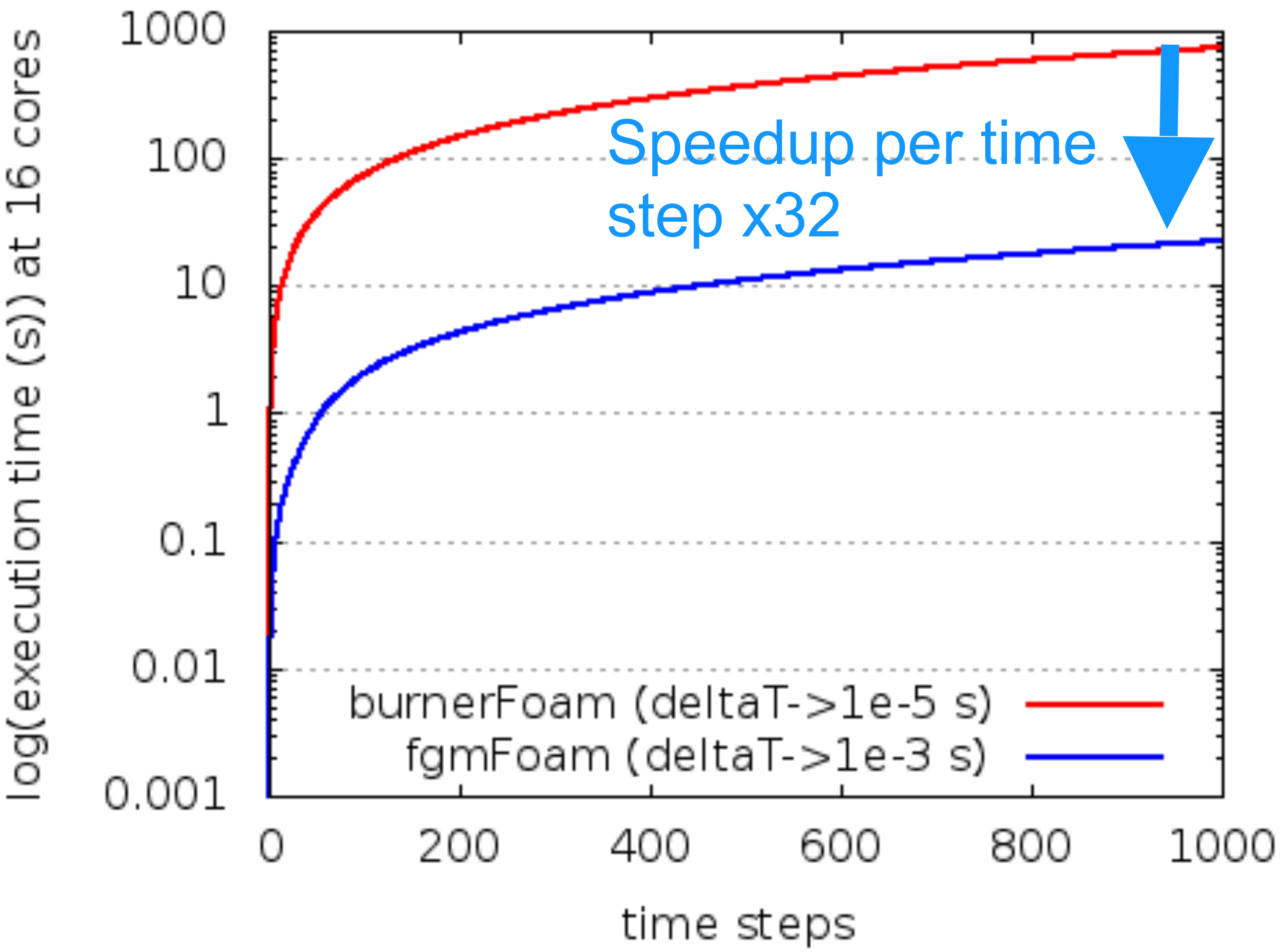
fgmFOAM solver

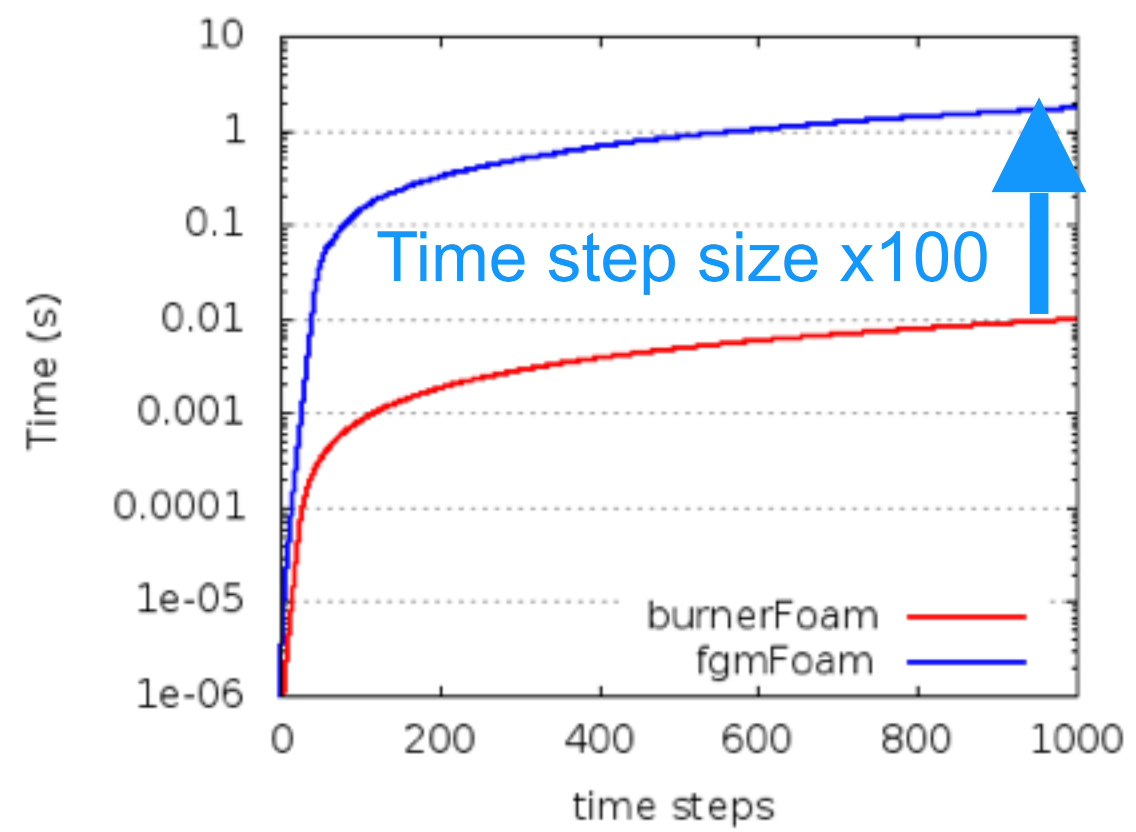
- Note FGM 'controlling' variables



fgmFOAM vs burnerFOAM: speedup

- Execution time per time step x32
- Time step size x100
  - Note use of the SIBS ODE solver (deprecated) with burnerFOAM





Computational requirements for flamelets (Once-only)

- CHEM1D for flameletes
  - (Also Cantera and Ember in other versions)

Pre-processing	Time		Storage	
	FGM3d	FGM4d	FGM3d	FGM4d
Flamelet generation	1h	4h	350 Mb	1.3 Gb
Triangulation	30"	2h	-	
Remapping (LUT)	3'	2h	90 Mb	2 Gb

i7-3820@3.6GHz, sequential

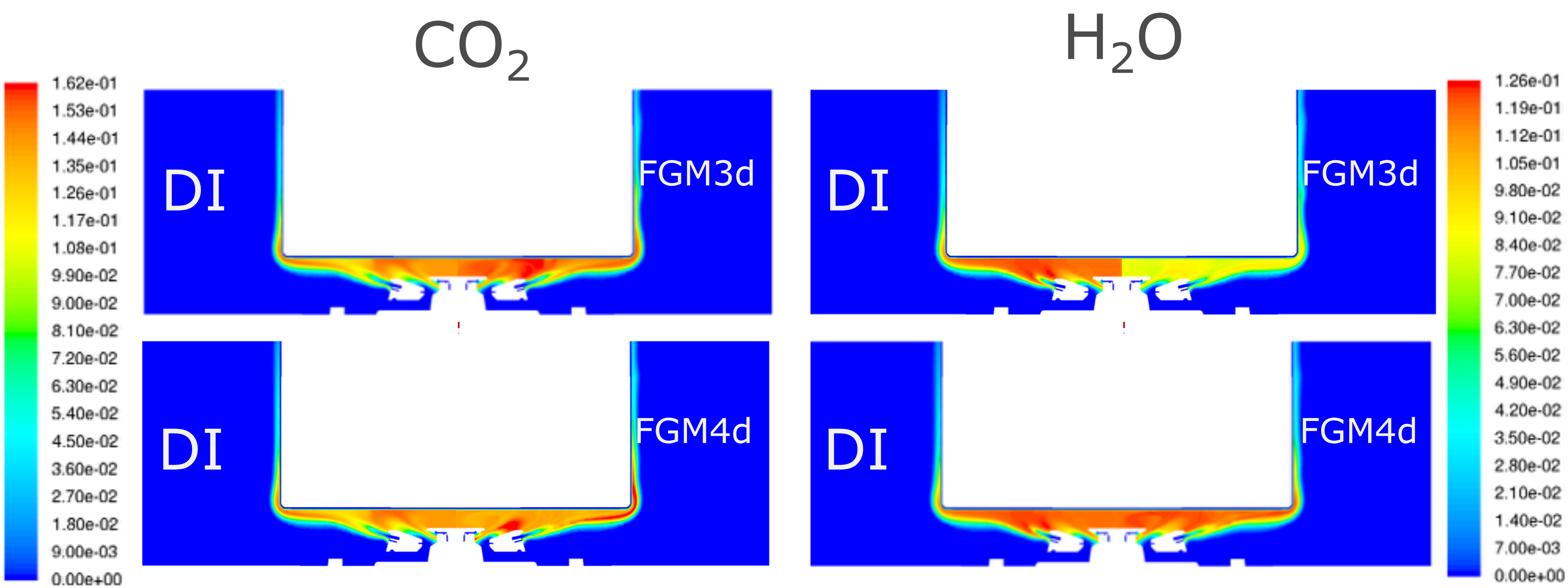
Conclusions

Conclusions and extensions

- New strategies for exploring thermochemical space successful
- Results for FGM
  - Good for temperature, reactants
  - Good for OH
  - Need improvement for main products (lumped under one reaction progress variable) and CO (not controlling variable)
  - Discrepancies often similar to those using reduced mechanism
- Idea for improvement: use a fourth manifold dimension (or more)

Extension to 4D: FGM4d

- Use CO as second progress variable
- (First one is still CO2+H20)
- Extension not difficult, due to remapping of manifold onto structured tables (but there are caveats)



Calculations on this slide made with ANSYS Fluent

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Support:

- Grants IPT-2011-1158-920000 (INNPACTO) and RTC-2014-1847-6 (RETOS-COLABORACIÓN) from Ministerio de Economía y Competitividad, Gobierno de España/ European Union
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