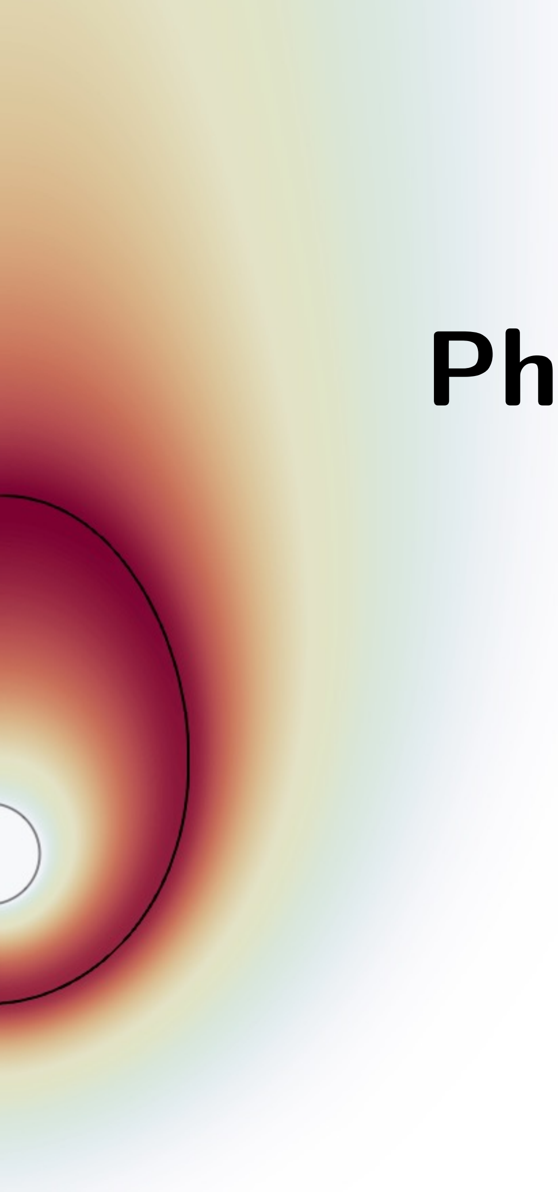


POLITECNICO MILANO 1863

Current State of Gas-Liquid Phase Change Modeling in Basilisk

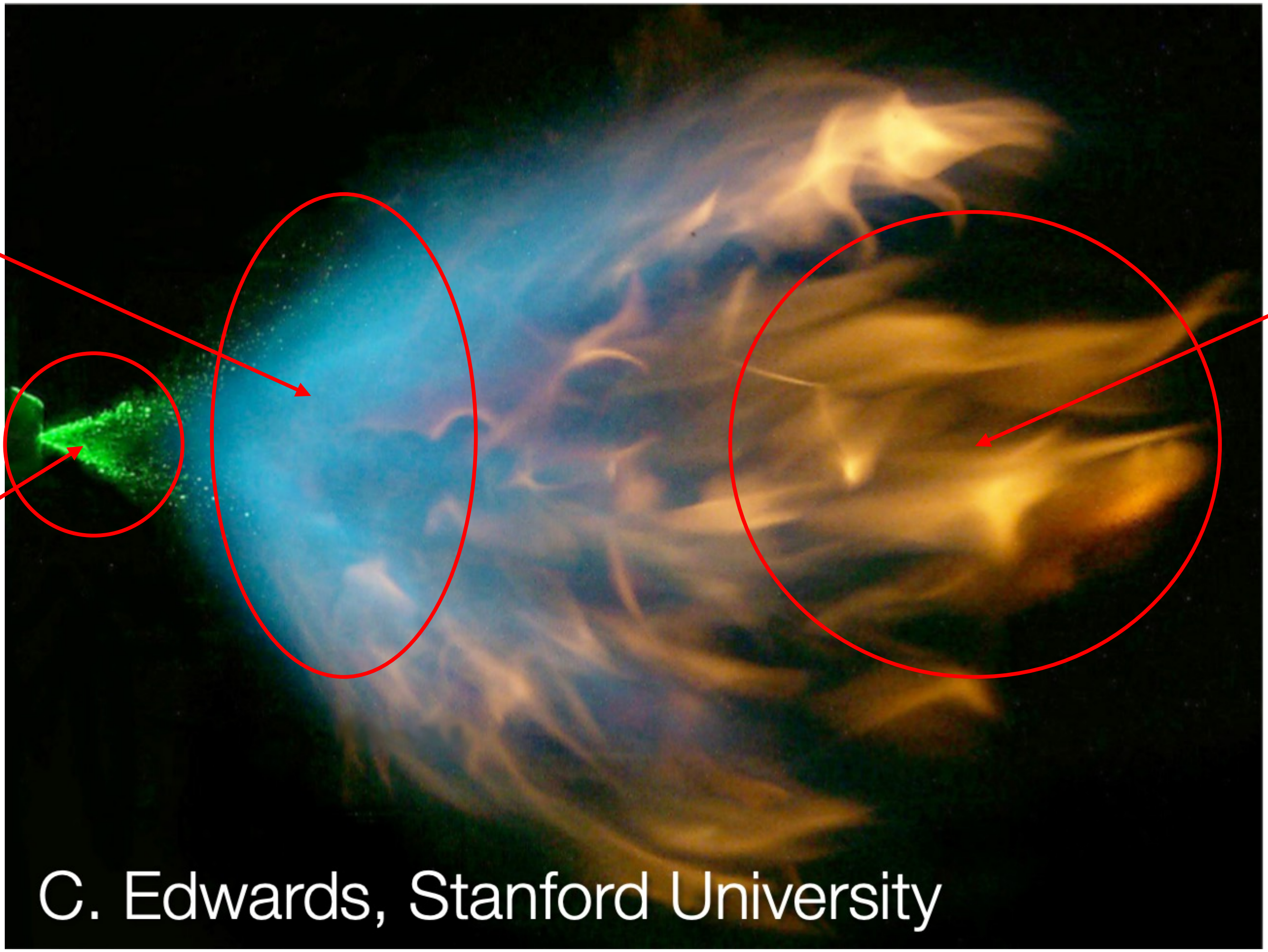
Edoardo Cipriano

CRECK Modeling Lab, Politecnico di Milano

BGUM 2025 – Oxford (UK)

The Spray Combustion Problem

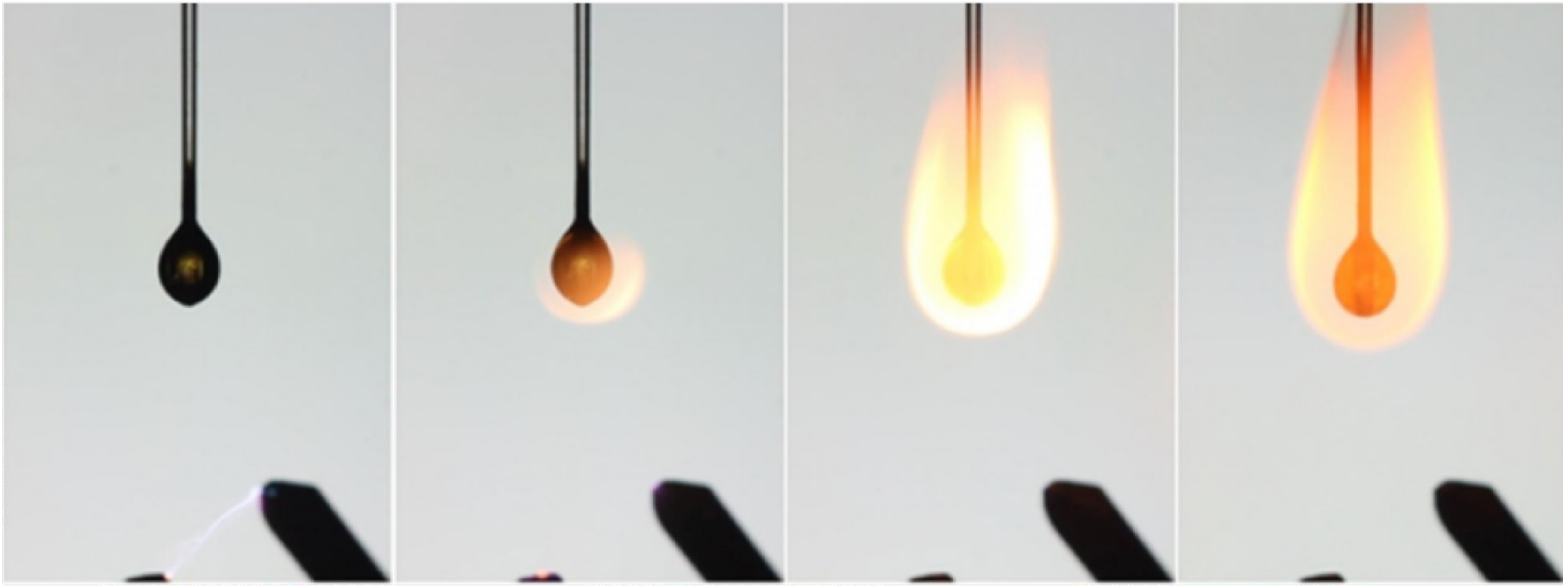
Strongly multiscale and multiphysics phenomenon



Isolated Droplet Configuration

We focus on a simplified configuration to:

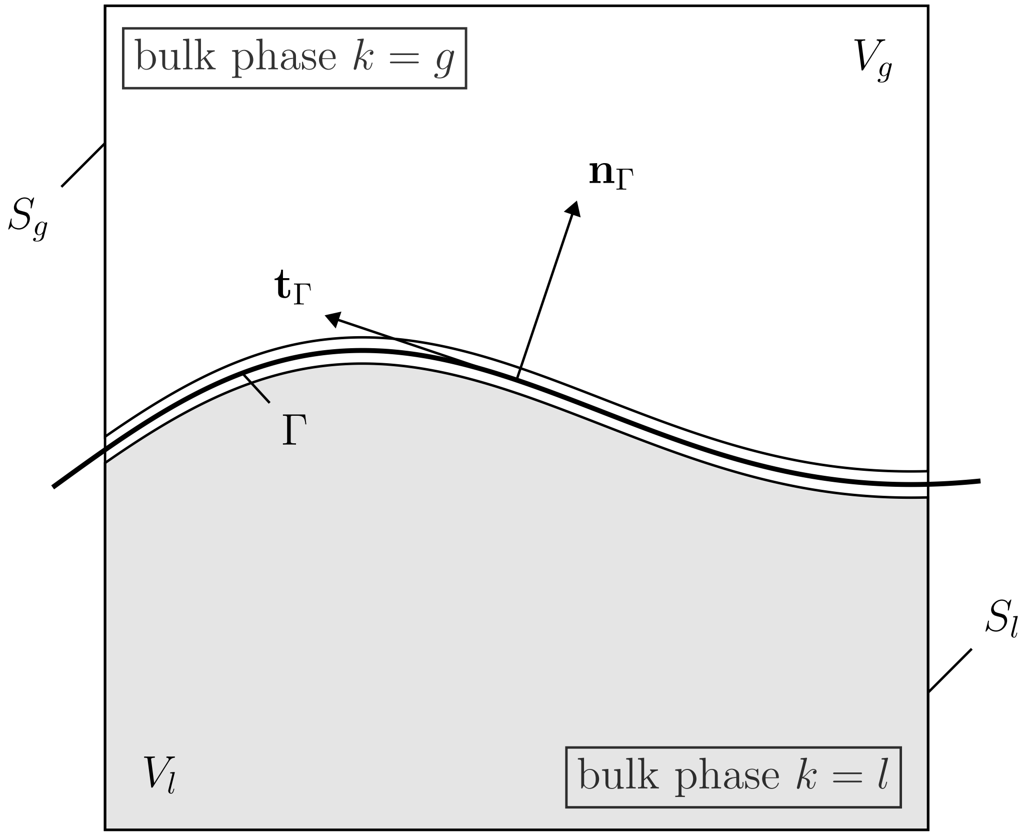
1. *Neglect interactions* between different droplets
2. *Refine our understanding* of evaporation and combustion processes
3. Develop *Sub-Grid-Scale correlations* for spray combustion models



Sankaranarayanan et al., *Fuel* (2019)

Bulk Phase Governing Equations

Valid for the bulk liquid or gas phases, not across the interface



Incompressible – Variable Properties – Combustion

$$\nabla \cdot \mathbf{u} = \beta \frac{DT}{Dt} + M_w \sum_{i=1}^{NS} \frac{1}{M_{w,i}} \frac{D\omega_i}{Dt}$$

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot (2\mu \mathbf{D}) - \nabla p_d + \mathbf{g} \cdot \mathbf{x} \nabla \rho$$

$$\rho \frac{D\omega_i}{Dt} = -\nabla \cdot \mathbf{j}_i + \dot{\Omega}_i$$

$$\rho c_p \frac{DT}{Dt} = -\nabla \cdot \mathbf{q} - \left(\sum_{i=1}^{NS} c_{p,i} \mathbf{j}_i \right) \cdot \nabla T - \sum_{i=1}^{NS} h_i \dot{\Omega}_i$$

Interface Jump Conditions

The control volume is a zero-thickness portion of the interface, with $[\boldsymbol{\phi}]_\Gamma = \boldsymbol{\phi_l} - \boldsymbol{\phi_g}$

Incompressible – Variable Properties – Combustion

$$[\mathbf{u}]_\Gamma \cdot \mathbf{n}_\Gamma = \dot{m}\,[1/\rho]_\Gamma$$

$$[p]_\Gamma = \sigma\kappa - \dot{m}\,[\mathbf{u}]_\Gamma \cdot \mathbf{n}_\Gamma$$

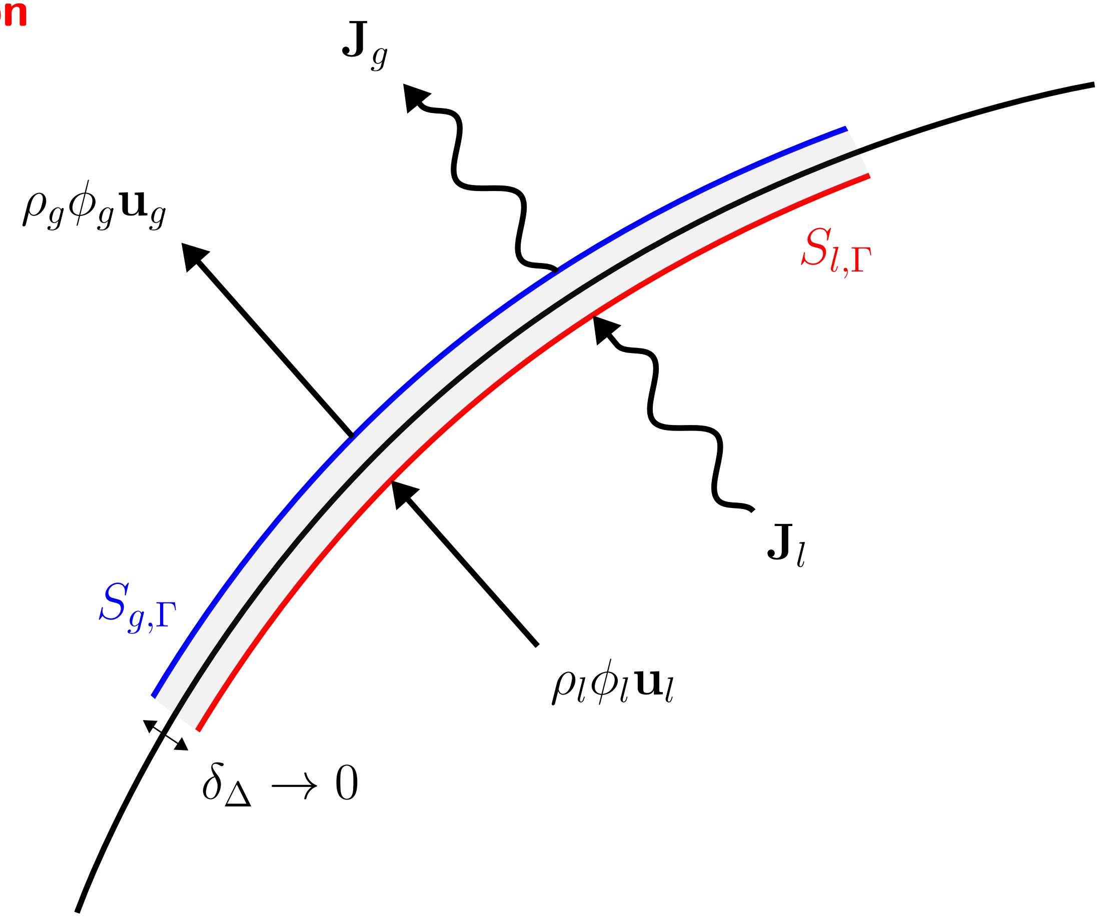
$$[\rho\,(\mathbf{u} - \mathbf{u}_\Gamma) \cdot \mathbf{n}_\Gamma]_\Gamma = 0$$

$$[\rho\omega_i\,(\mathbf{u} - \mathbf{u}_\Gamma) \cdot \mathbf{n}_\Gamma + \mathbf{j}_i \cdot \mathbf{n}_\Gamma]_\Gamma = 0$$

$$[\lambda\nabla T \cdot \mathbf{n}_\Gamma]_\Gamma = \sum_{i=1}^{NLS} \dot{m}_i\,[h_i]_\Gamma + \dot{q}_{rad}$$

$$[f_i]_\Gamma = 0$$

$$[T]_\Gamma = 0$$



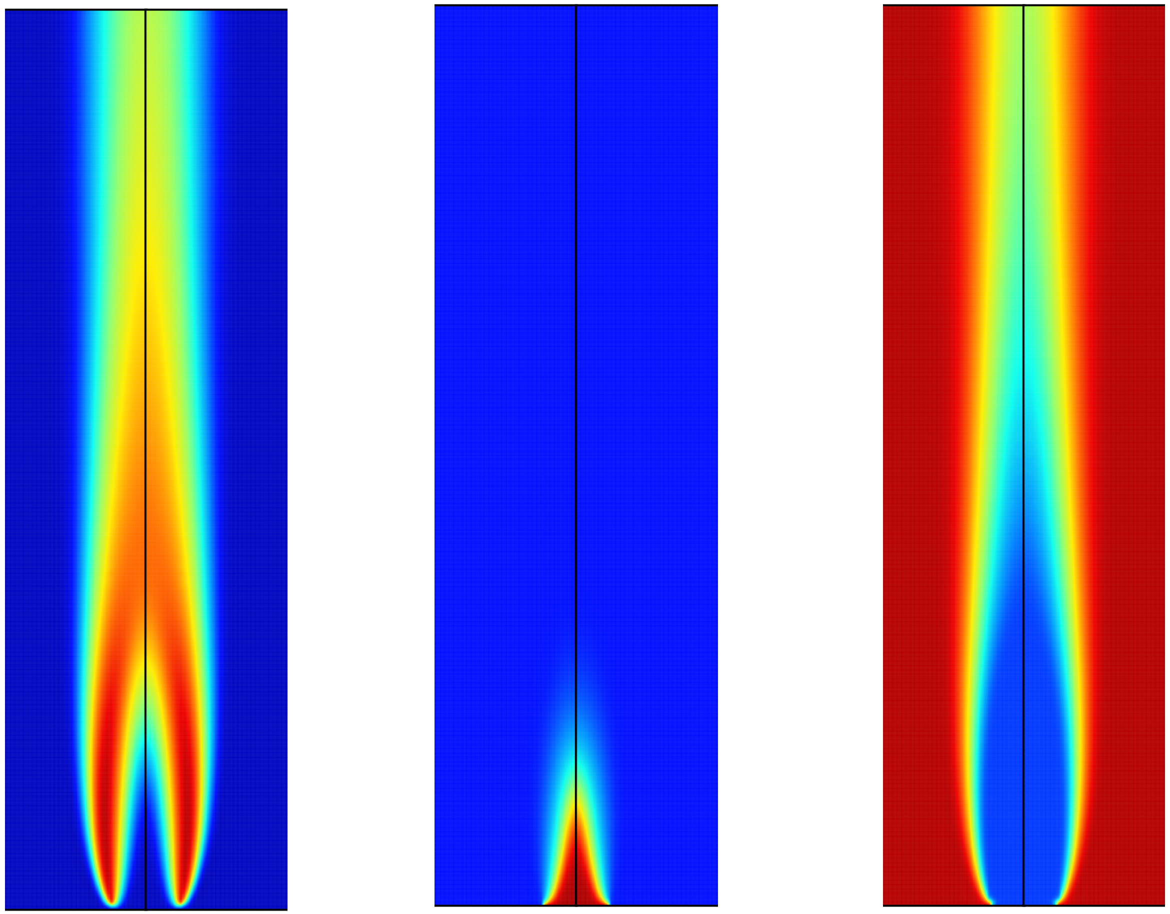
Challenges of the Numerical Solution

Numerically, simulations of phase change and combustion are hindered by several factors:

Combustion

- Density Changes
- Multicomponent
- Diffusion Models
- Radiation
- Coupling and Non-linearity

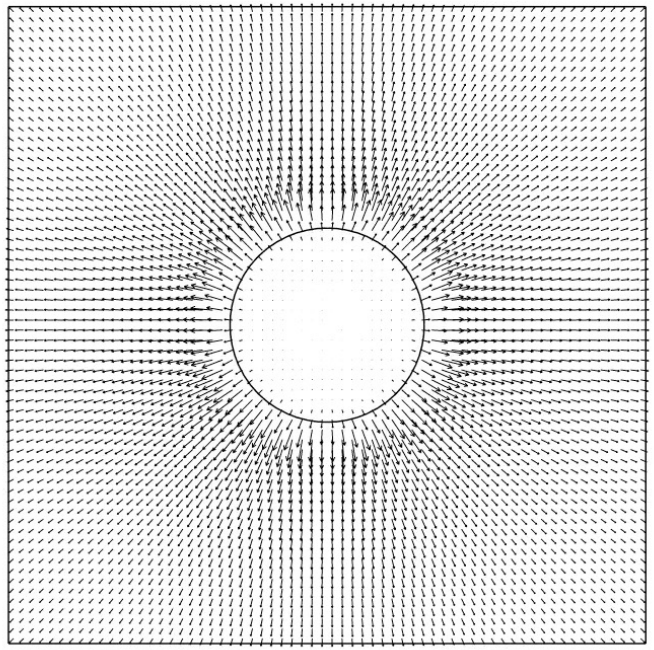
Temperature Hydrogen Oxygen



Hydrogen co-flow flame using Basilisk

Challenges of the Numerical Solution

Numerically, simulations of phase change and combustion are hindered by several factors:



Stefan flow from a Vaporizing Droplet

Phase Change

- Gas-Liquid boundary conditions
- Interface velocity
- Localized expansion

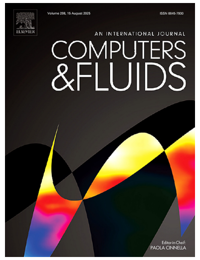
Phase Change Contributions

Available open-source phase change models in Basilisk

A phase-change model for diffusion-driven mass transfer problems in incompressible two-phase flows

G.Gennari, R. Jefferson-Loveday, S.J. Pickering (2022)

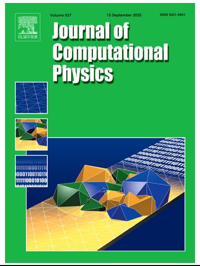
Shifted Expansion



A consistent volume-of-fluid approach for direct numerical simulation of the aerodynamic breakup of a vaporizing drop

B. Boyd, Y. Ling (2023)

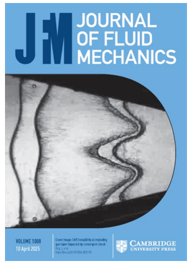
Consistent



Multicomponent droplet evaporation in a geometric volume-of-fluid framework

E. Cipriano, A.E. Saufi,, A. Frassoldati, T. Faravelli, S. Popinet, A. Cuoci (2024)

Two-Velocities



Direct numerical simulation of nucleate boiling with a resolved microlayer and conjugate heat transfer

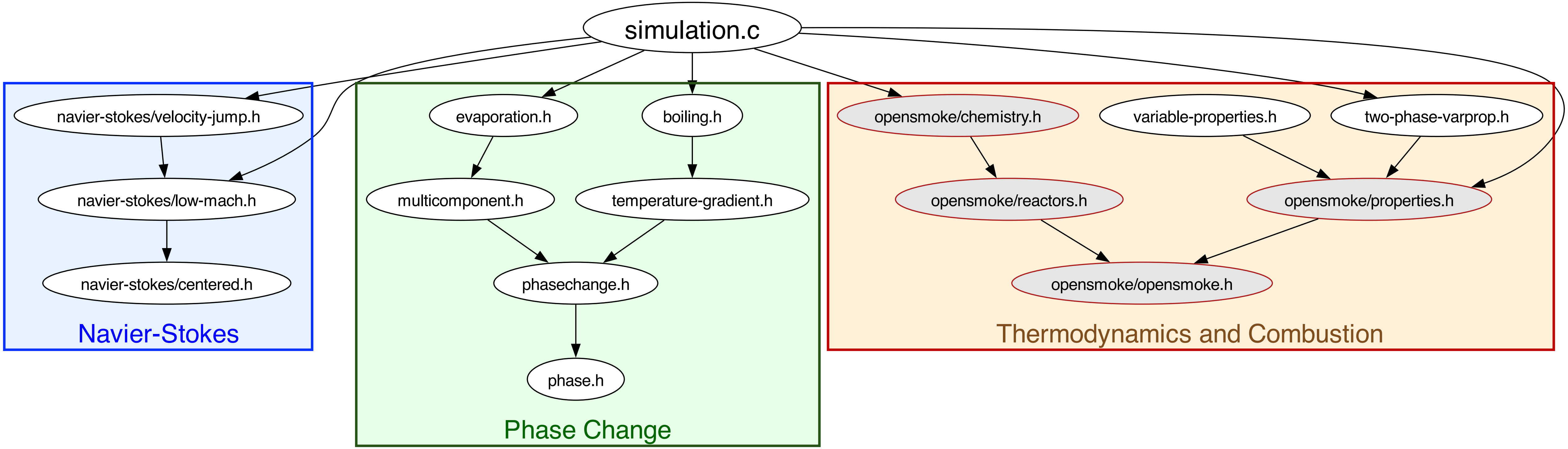
T. Long, J. Pan, E. Cipriano, M. Bucci, S. Zaleski (2025, Under Review)

GFM

How can we merge the core features of these models in a single, unified framework?

Structure of the Code

The connections between the main headers.

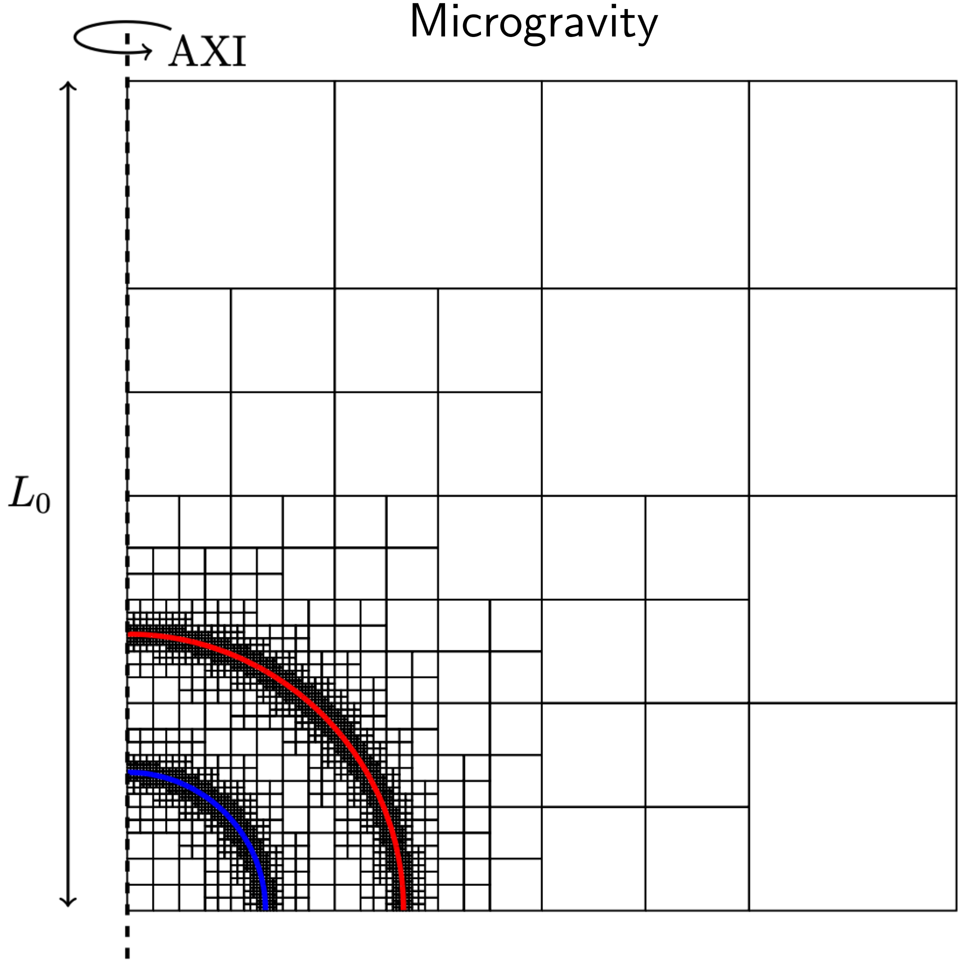


Application to
Droplet Combustion Problems

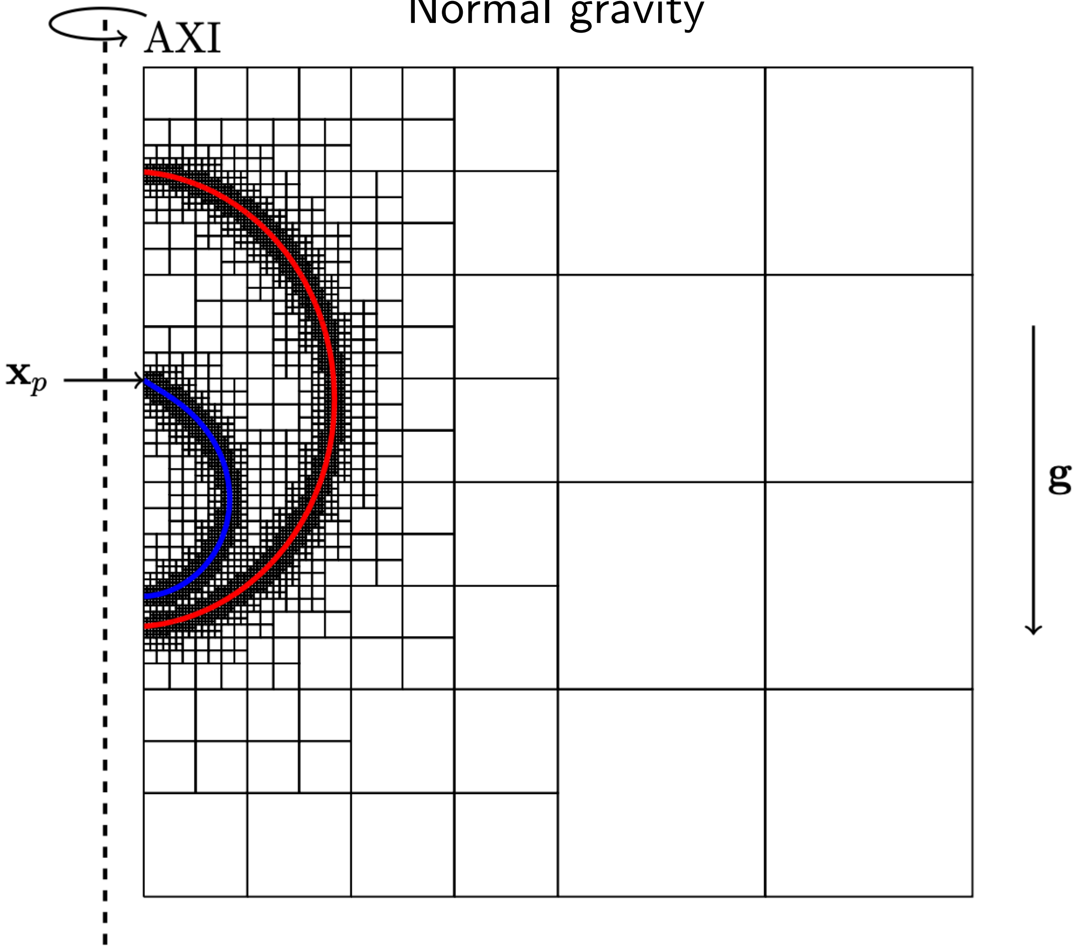
Combustion Simulation Setup

Simulation setup for droplet combustion problems in microgravity and in normal gravity conditions

Microgravity



Normal gravity



Combustion Simulation Setup

Two-step kinetics to reduce the computational time as much as possible.

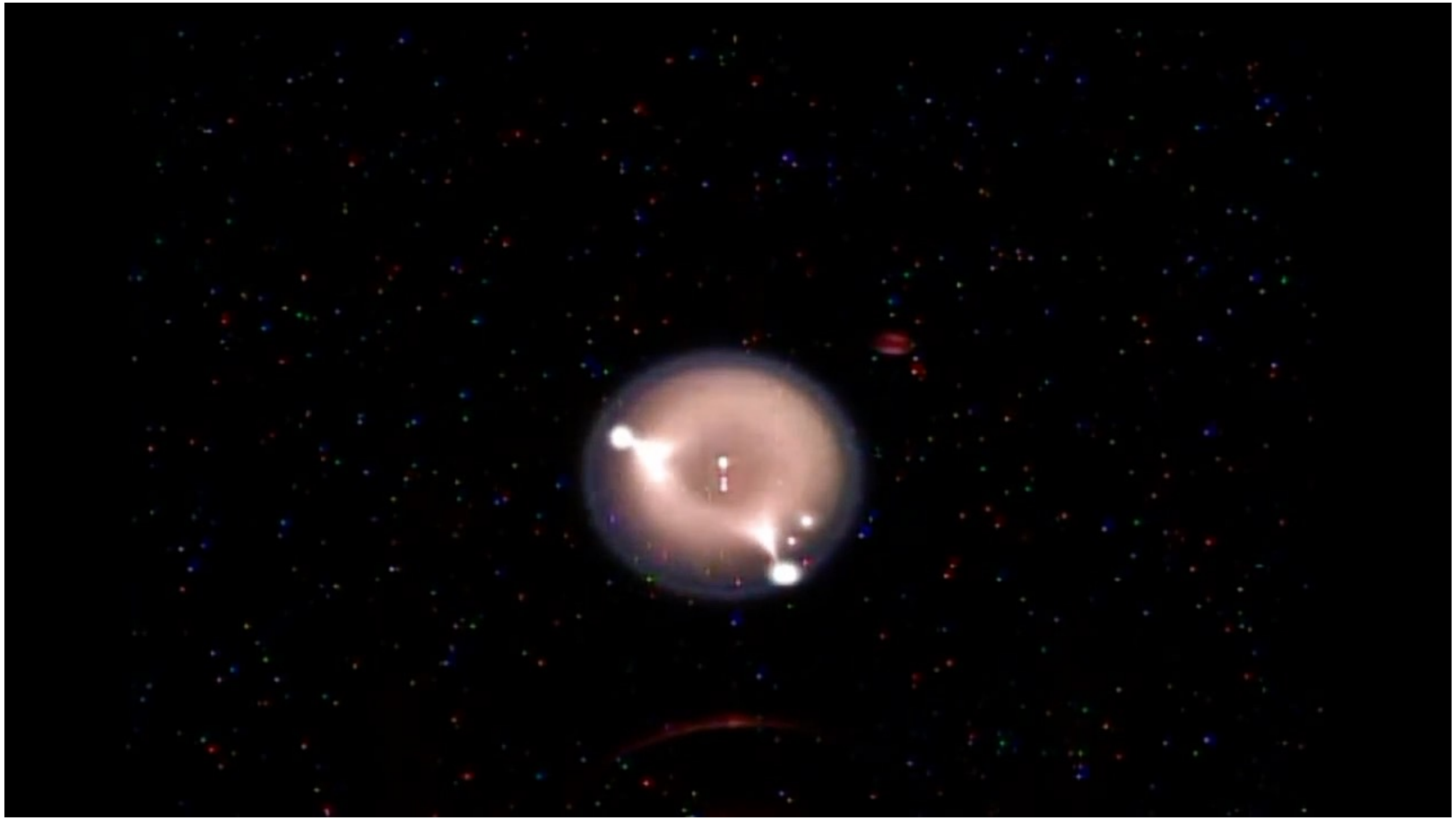
$$\mathrm{C}_n\mathrm{H}_m + \left(\frac{n}{2} + \frac{m}{4}\right)\mathrm{O}_2 \xrightarrow{k_1} \mathrm{nCO} + \frac{m}{2}\mathrm{H}_2\mathrm{O}$$

$$\mathrm{CO} + \frac{1}{2}\,\mathrm{O}_2 \xrightleftharpoons{k_2} \mathrm{CO}_2$$

Westbrook and Dryer, *Combustion Science and Technology* (1981)

How does a droplet burn in microgravity?

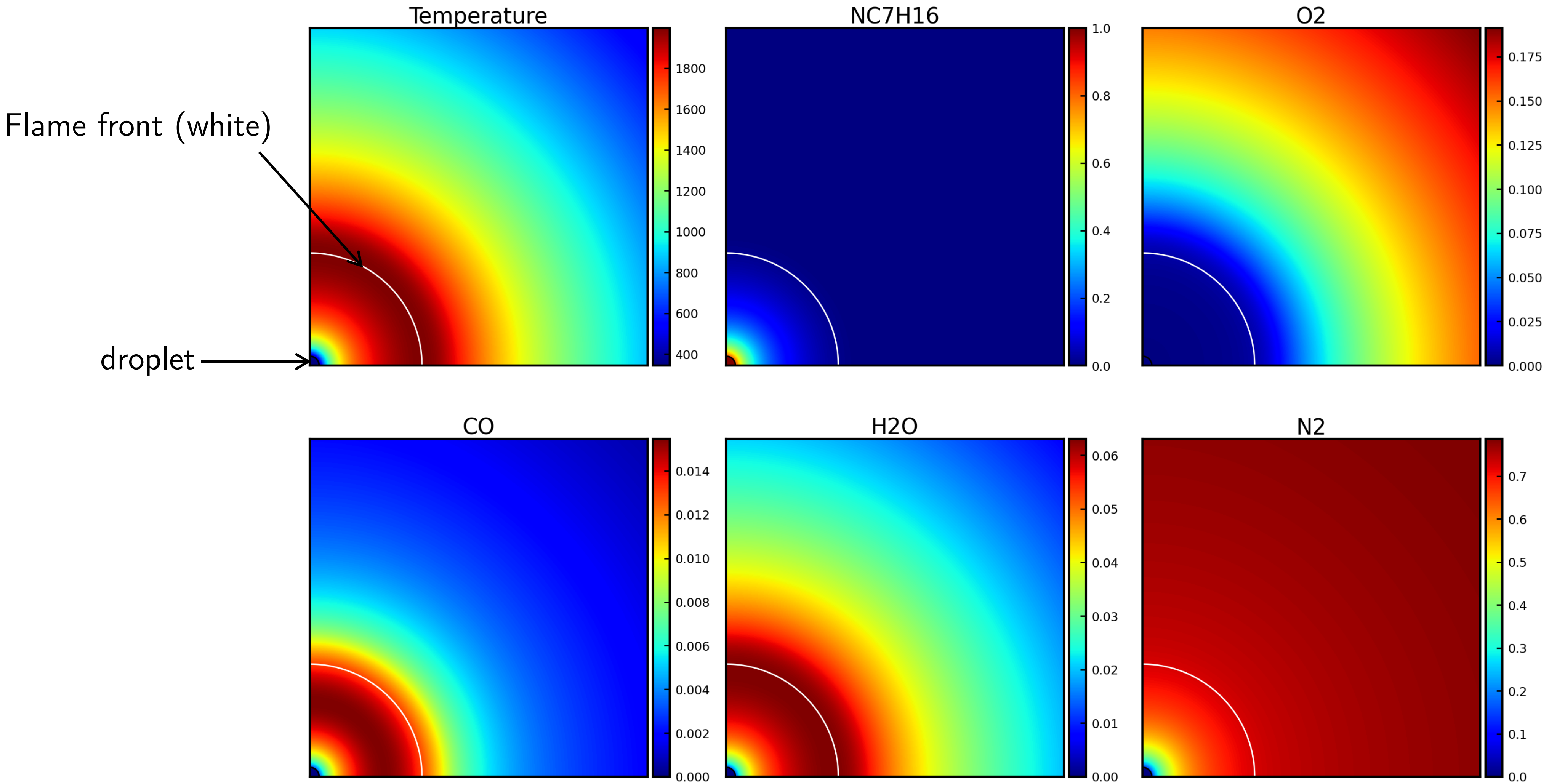
Experiment on the International Space Station



Dietrich et al., *Microgravity Sceience and Technology* (2014)

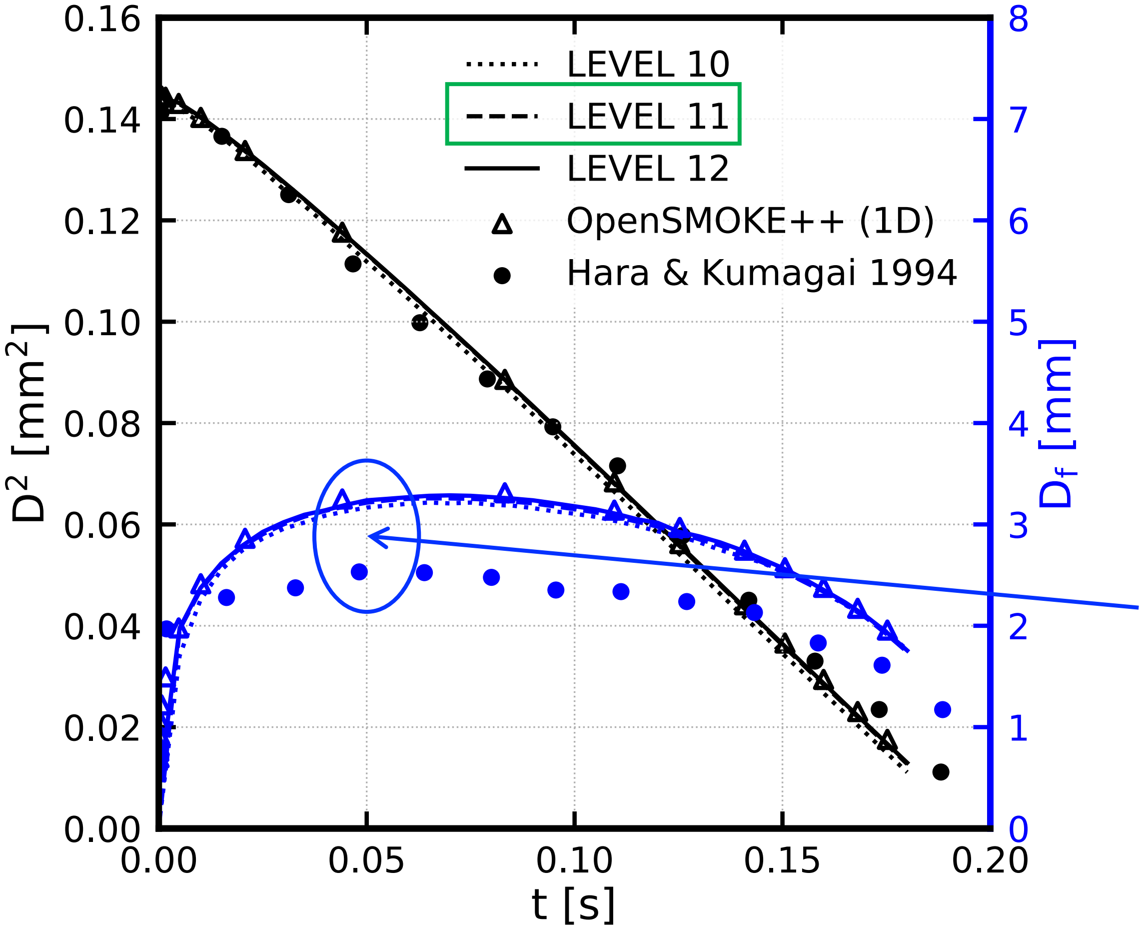
N-Heptane Combustion in Microgravity

Maps of the temperature and chemical species mass fractions fields



N-Heptane Combustion in Microgravity

Grid independence study, comparison with experimental data and with a 1D model



+ Convergence on the D^2
+ Correct burning rates
+ Matching 1D and experiments

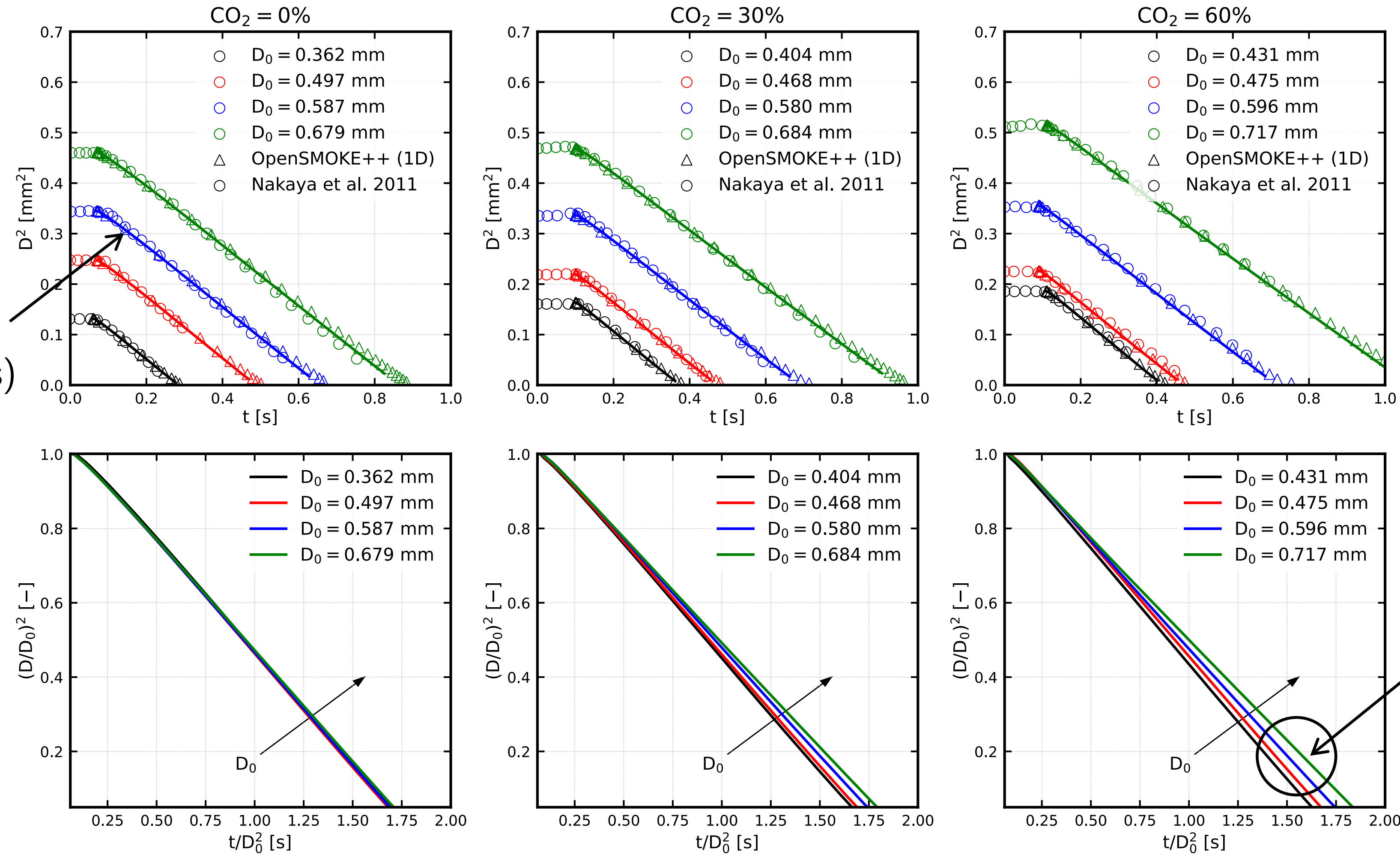
- Overestimation of the *flame front*
- No soot formation (simple kinetics)

Hara and Kumagai., *Symposium Int. on Combustion*, (1996) – **Cuoci et al.**, *Journal of Comp. Science* (2024).

Ethanol Droplet in Microgravity

Effect of the initial diameter, environment composition, and radiation

Comparison with experiments (circles) and 1D model (triangles)

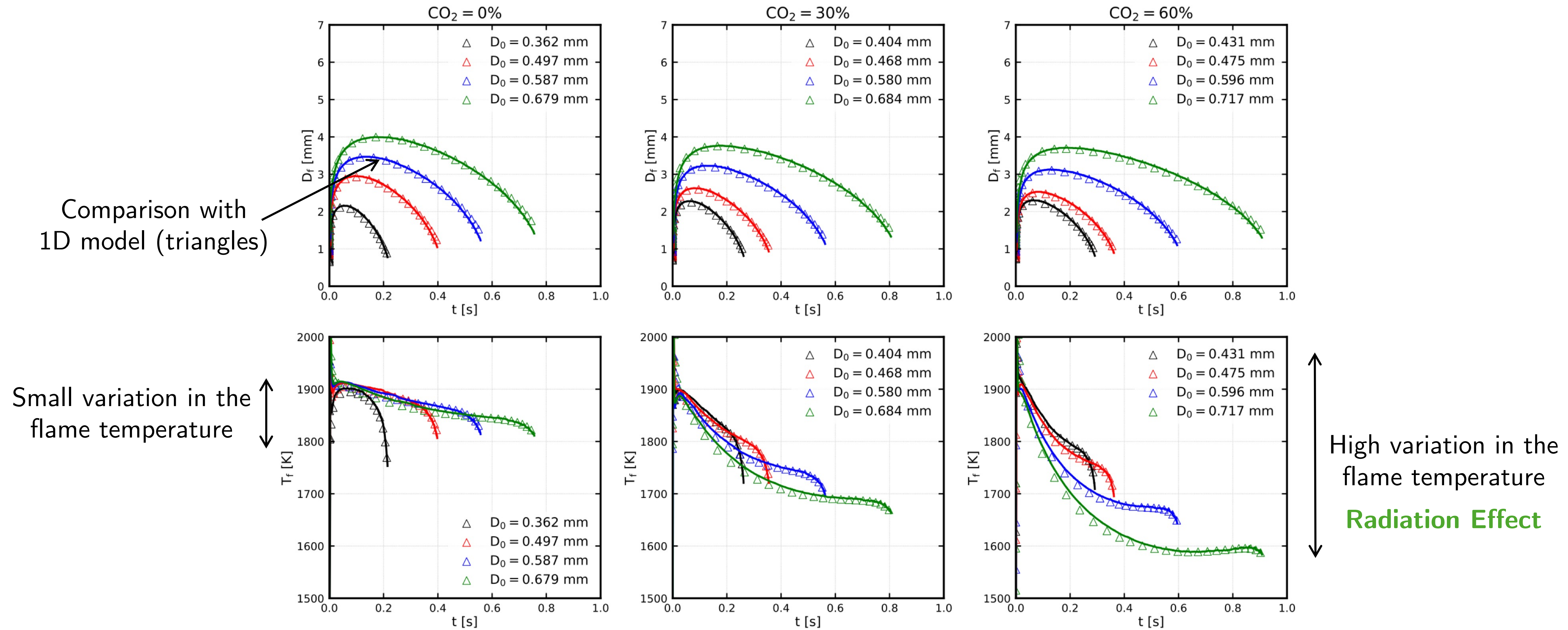


Increasing the CO2, the initial diameter changes the slope

Nakaya et al., *PROCI* (2011)

Ethanol Droplet in Microgravity

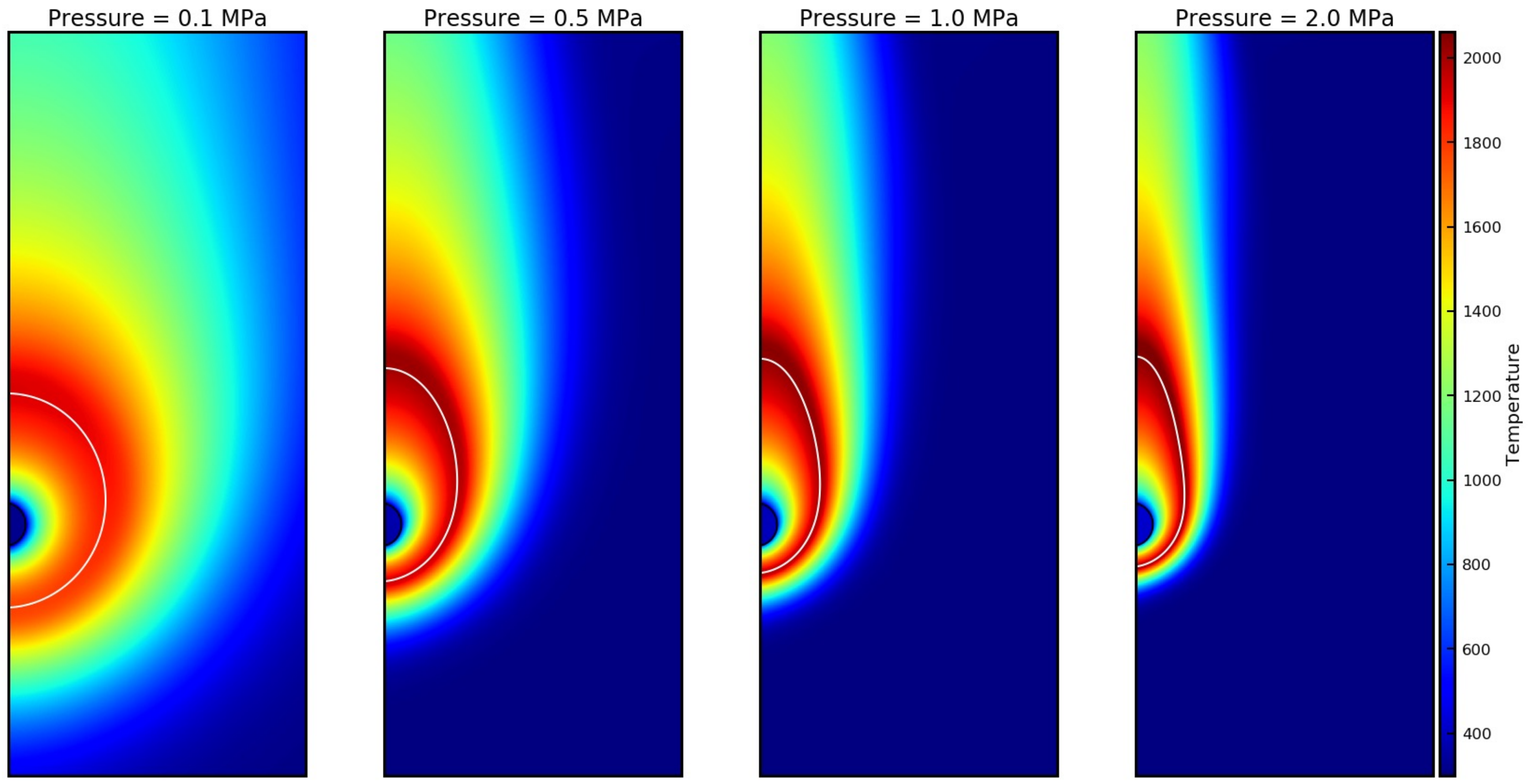
Effect of the initial diameter, environment composition, and radiation



Nakaya et al., *PROCI* (2011)

Combustion of Methanol Droplets in Normal Gravity

Evolution of the flame (temperature) at different pressures



Pressure

Flame stretching

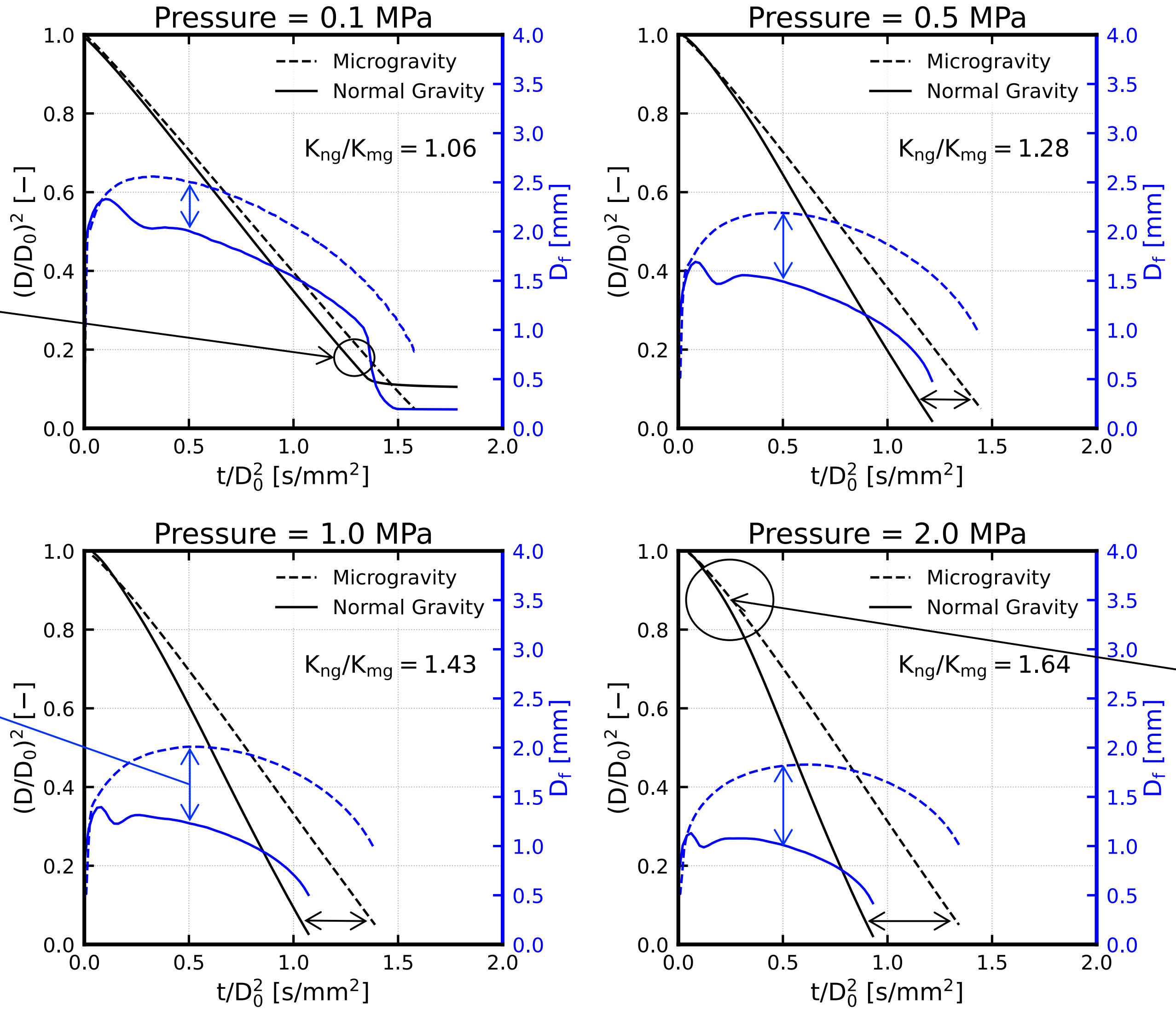
Combustion of Methanol Droplets in Normal Gravity

Measuring the displacement from the microgravity conditions

Linear, 6% deviation from microgravity

Flame front closer to the surface

Neglecting water condensation

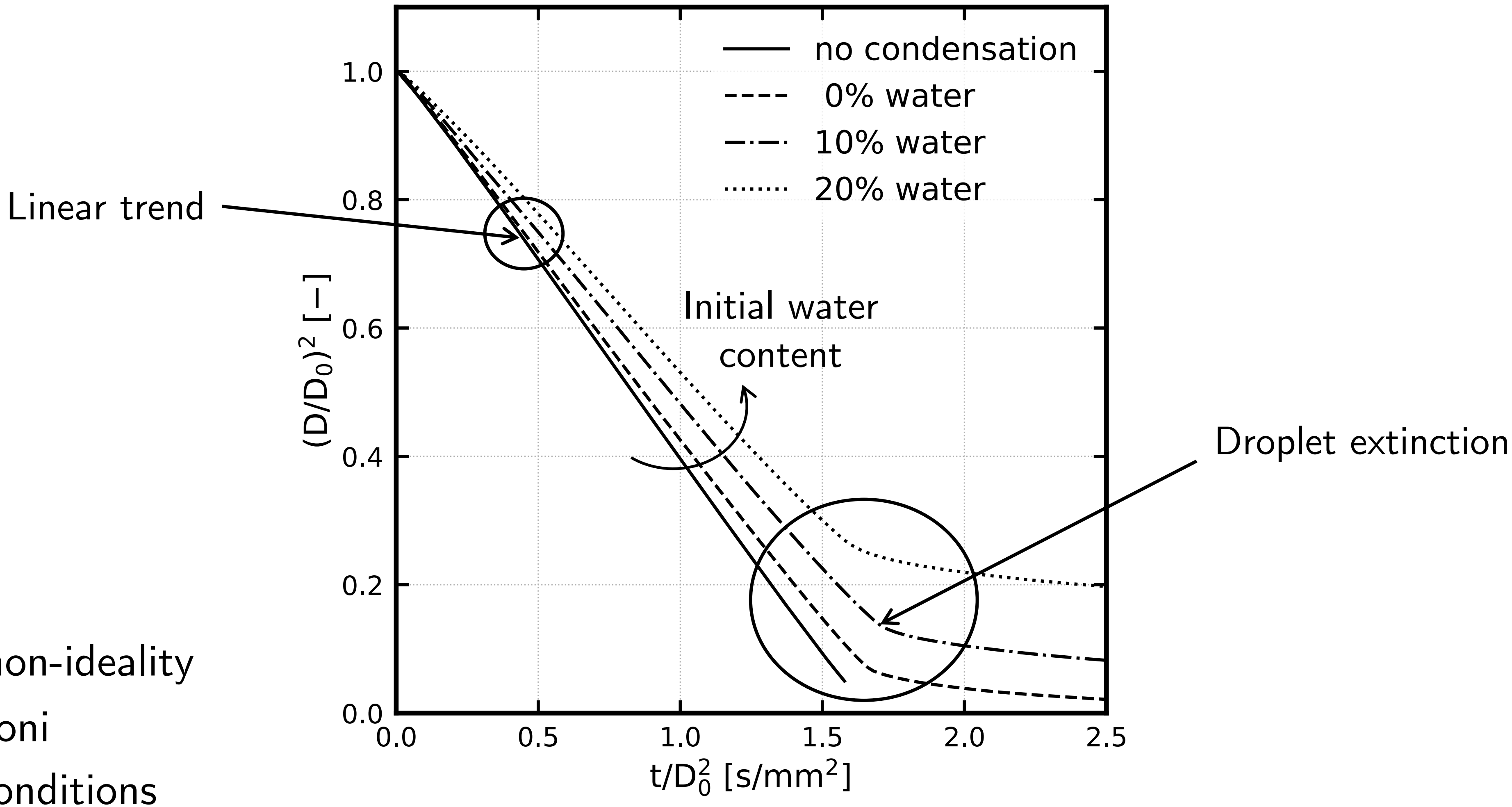


P= 5 atm: 28% deviation
P=10 atm: 43% deviation
P=20 atm: 64% deviation

Initial unsteadiness

Water Condensation Effects

During the combustion of methanol droplets in microgravity conditions



- Liquid non-ideality
- Marangoni
- Initial conditions

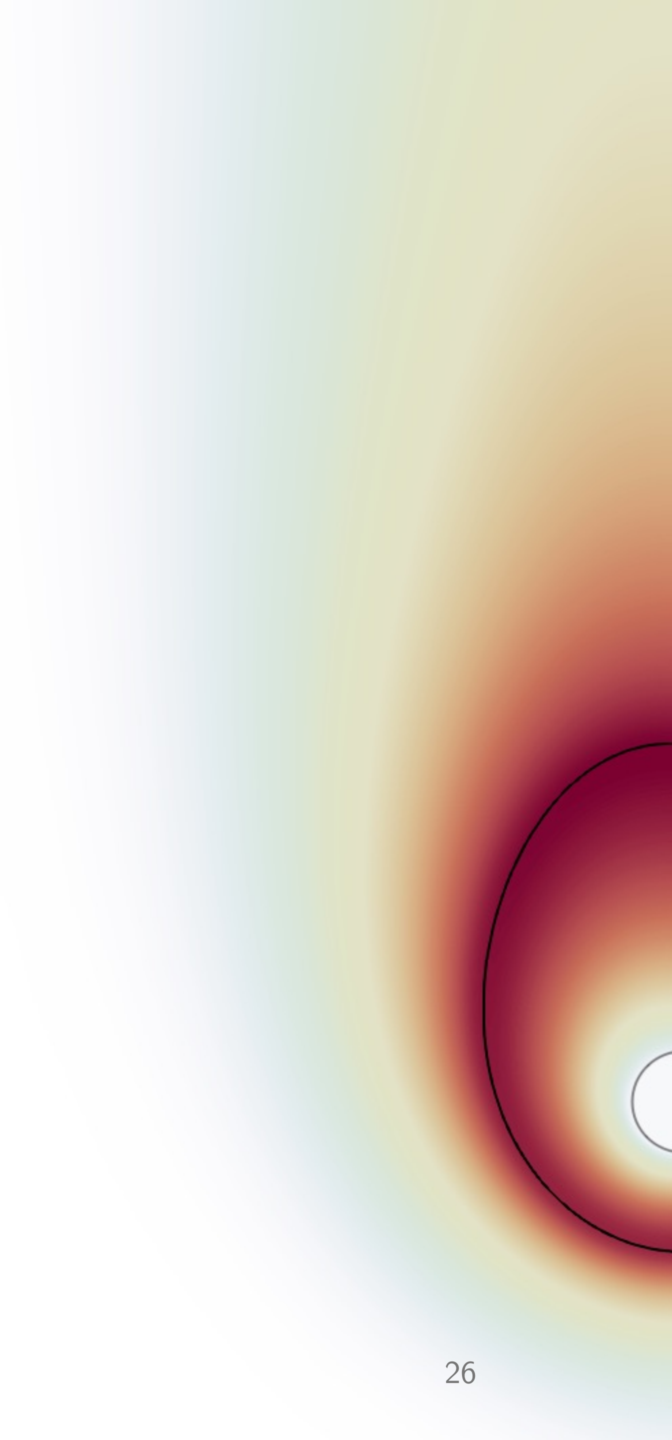
Conclusions

What did I do?

1. Unified framework for phase change
2. Variable material properties
3. Combustion chemistry
4. Application to droplet combustion problems

Next Steps

1. The new version will be available in September
2. Introduce Embed and CHT
3. Introduce Marangoni effect
4. Explore new configurations



Thank you for your attention.