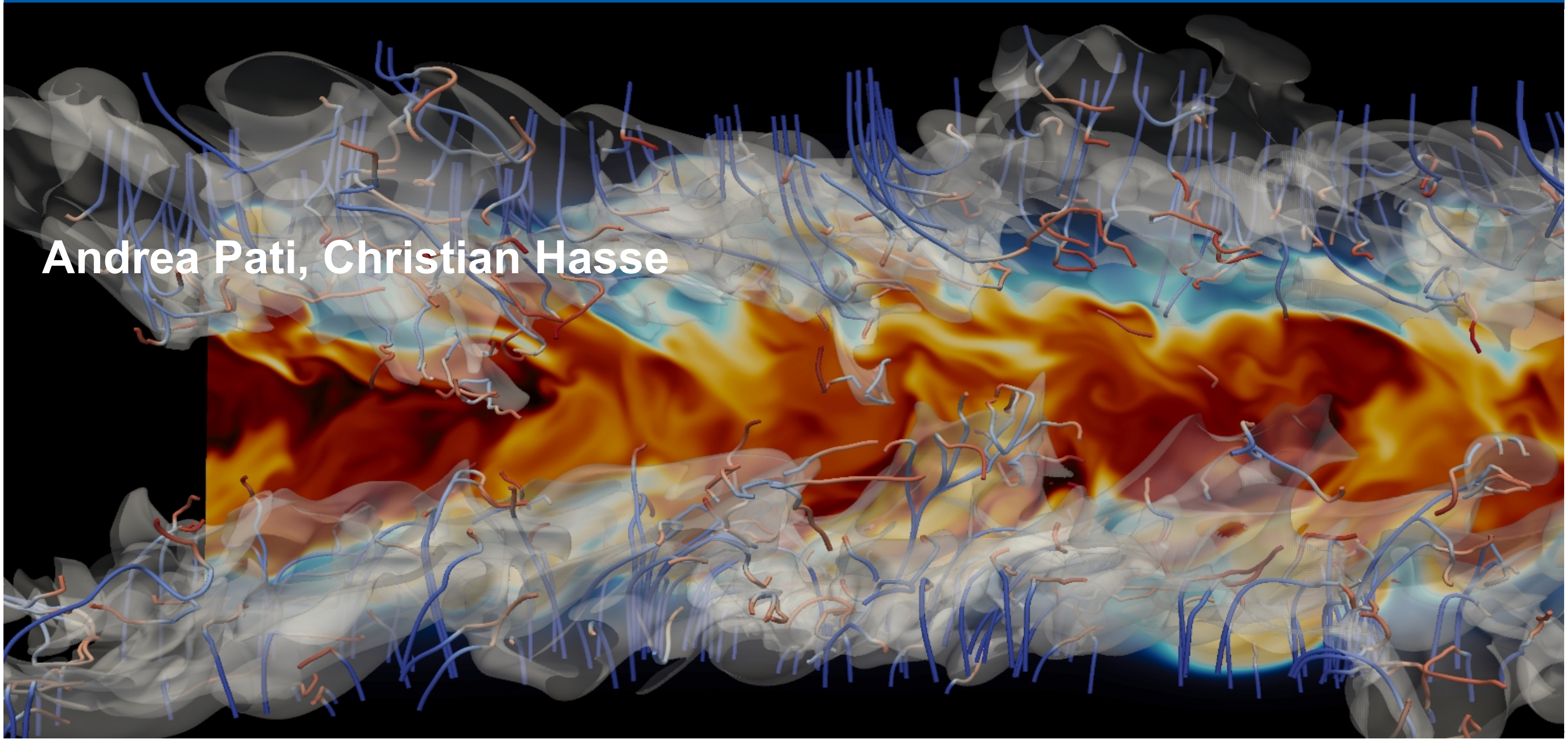
3D spray simulation using advanced intra-droplet and interface modeling

TU Darmstadt
Mechanical Engineering – Simulation of reactive Thermo-Fluid Systems

TECHNISCHE UNIVERSITÄT DARMSTADT

STFS
Simulation of reactive Thermo-Fluid Systems

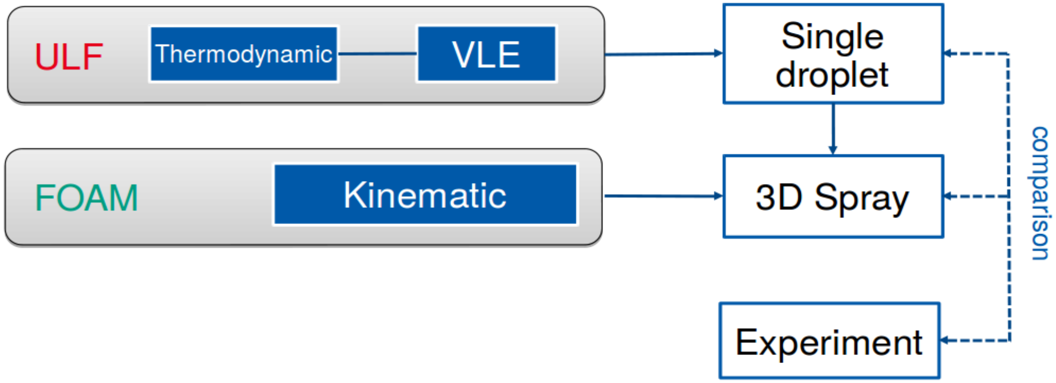


Andrea Pati, Christian Hasse

Agenda

TECHNISCHE UNIVERSITÄT DARMSTADT

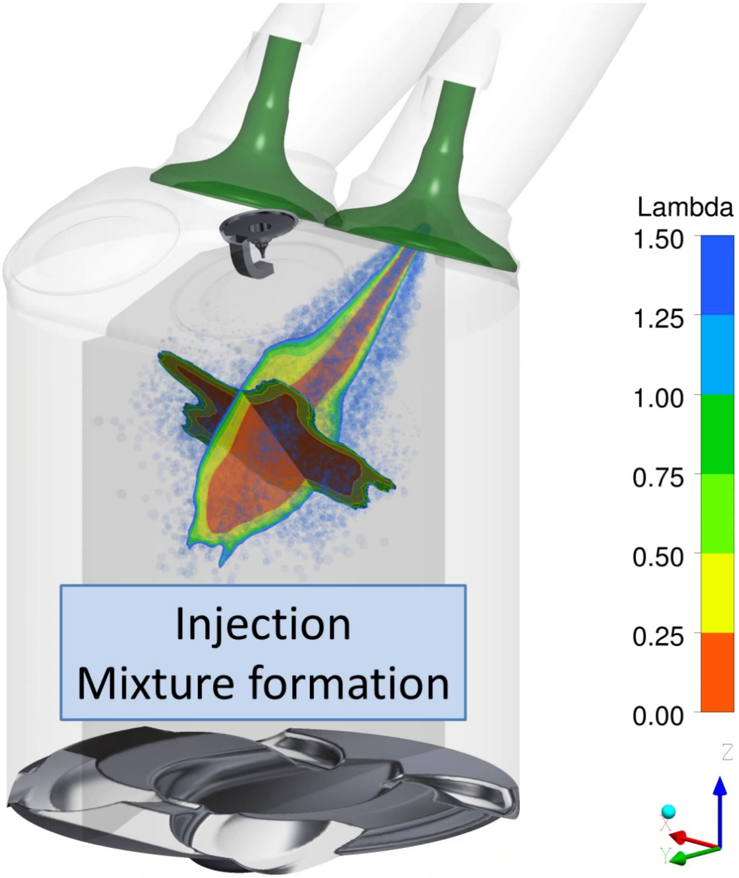
- **Introduction**
- ULF single droplet
- Foam coupling
- Verification
- Spray A
- Conclusion



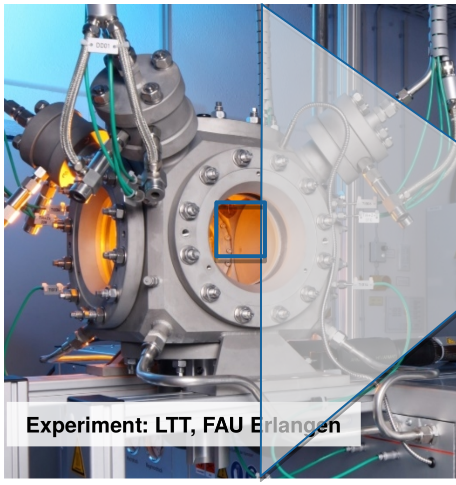
Introduction

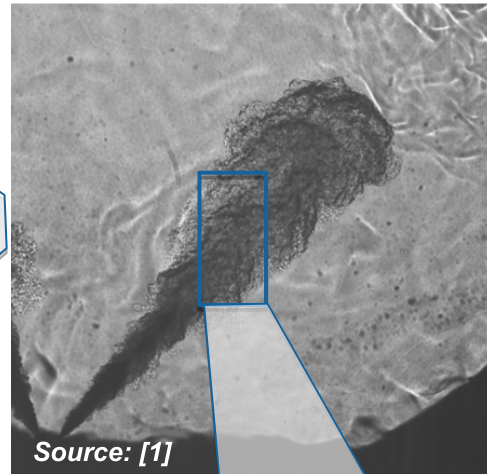
- Spray evaporation is first step in air/fuel mixture formation

- Spray evolution determines conditions for the following steps
  - Mixture formation in gas phase
  - Flame propagation
  - Pollutant formation



Evaporation / Mixing Sub-Critical

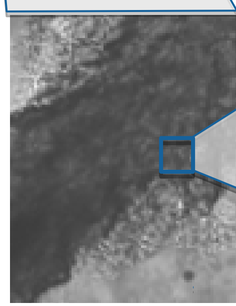


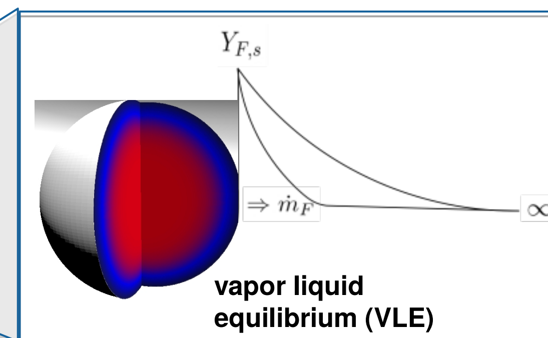


- Single droplets can be identified in high pressure sprays
- Systematic approach: From single droplets to high pressure spray

- Multi component mixture
- Thermodynamics at interface

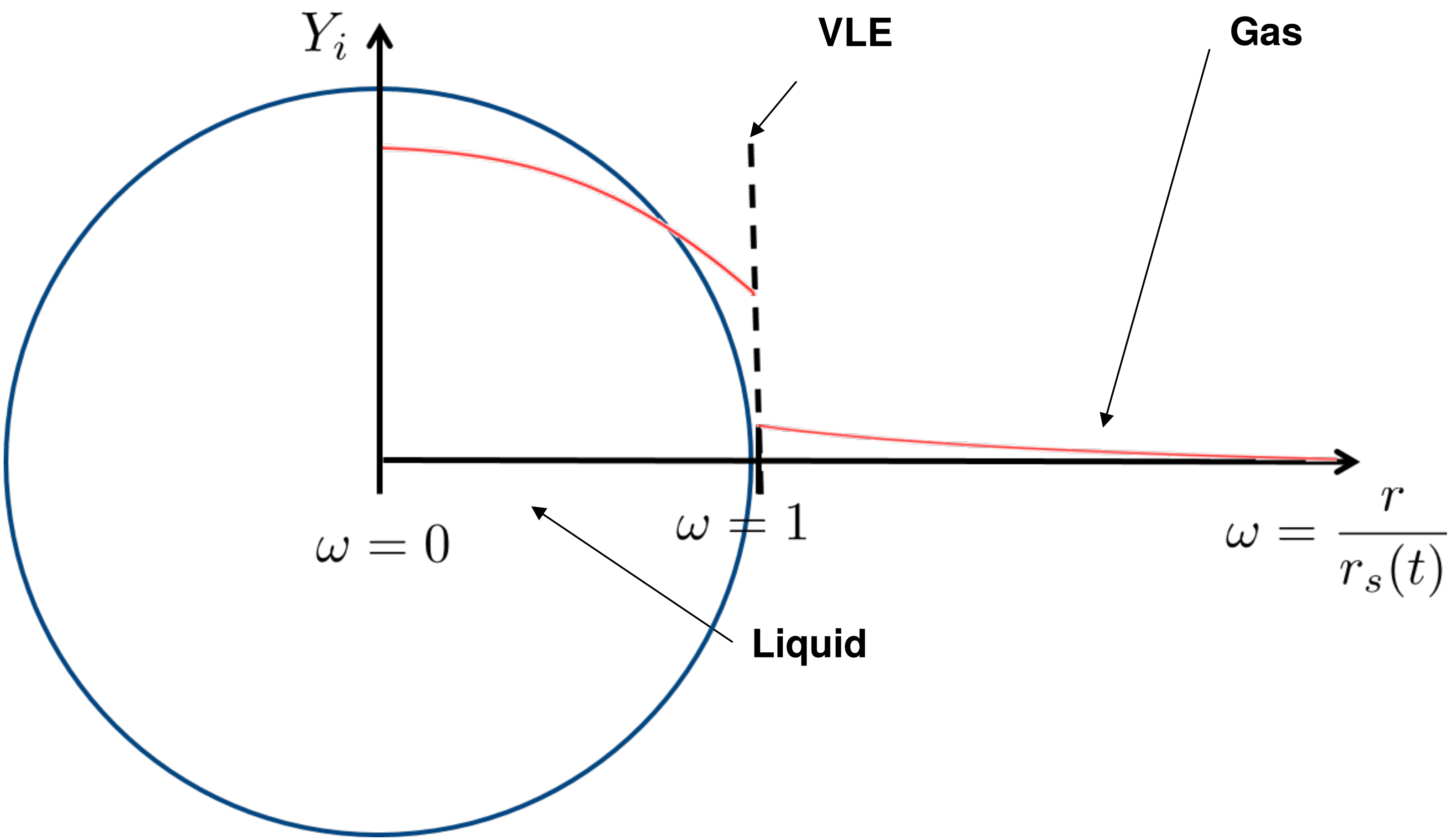
→ Vapor Liquid Equilibrium (VLE)



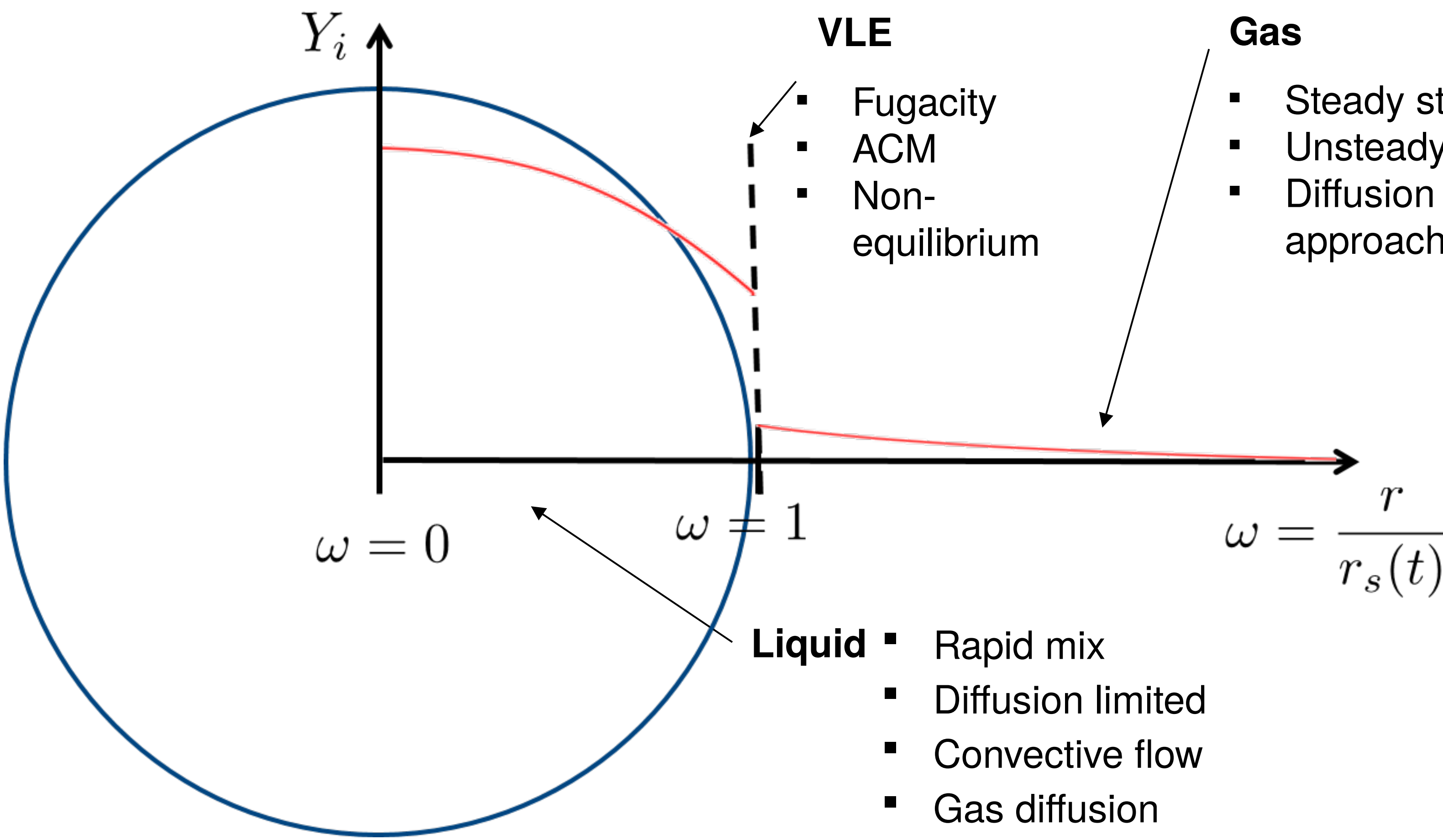


[1]: L. Weiss, A. Peter, M. Wensing, „ Diesel Spray characterization with Schlieren-MiDiesel Spray characterization with Schlieren-Mie Technique“, 18th International Symposium on the Application of Laser and Imaging Techniques to Fluid Mechanics, Lisbon 2016

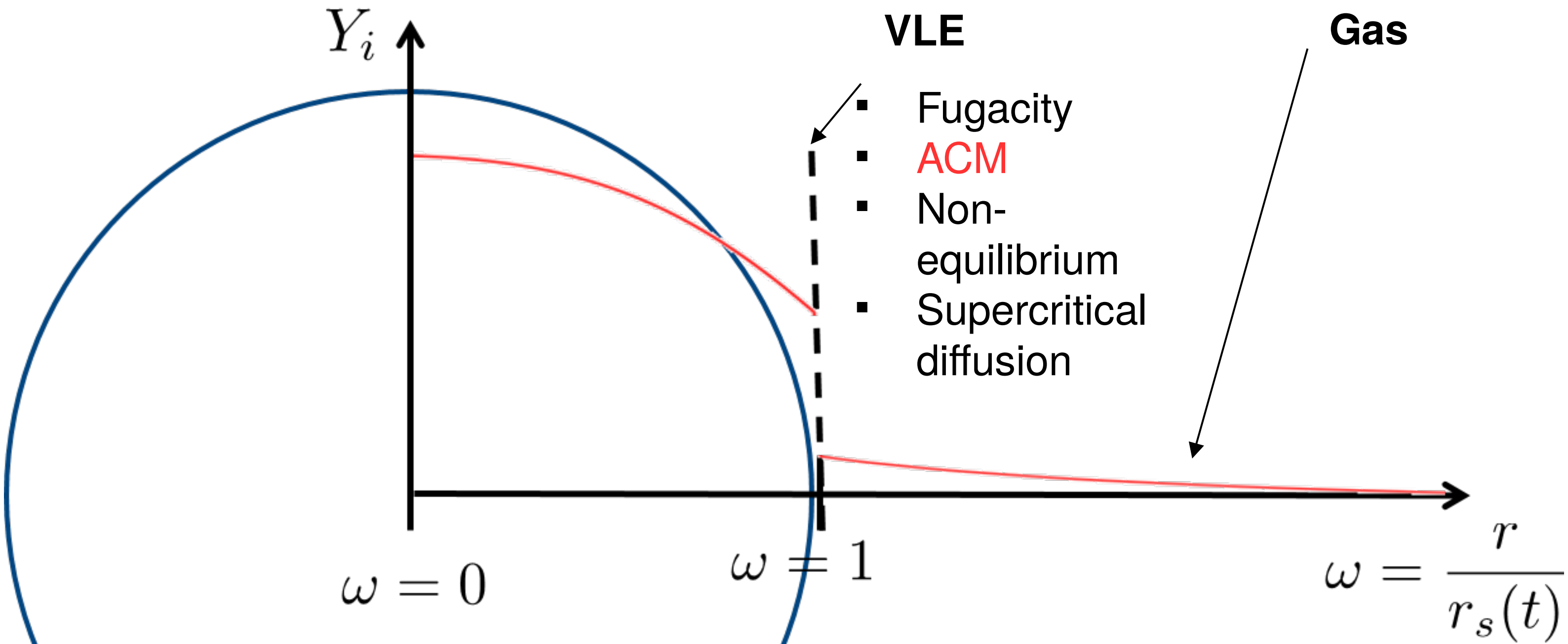
Droplet modeling



Droplet modeling



Droplet modeling

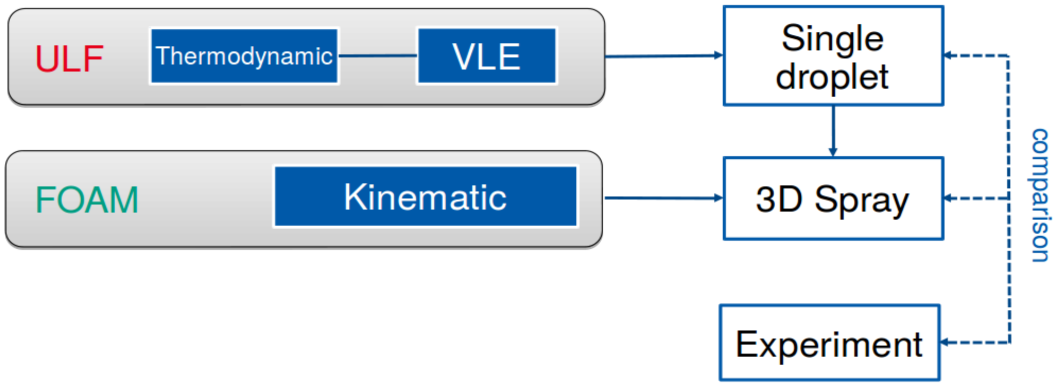


$$X_i^v = \frac{\gamma_i^l X_i^l f_i^0}{\varphi_i^v p} = X_i^l \frac{p_i^0}{p} \frac{\gamma_i^l \varphi_i^0}{\varphi_i^v} \mathrm{Poy}_i$$

Agenda

TECHNISCHE UNIVERSITÄT DARMSTADT

- Introduction
- **ULF single droplet**
- Foam coupling
- Validation
- Spray A
- Conclusion

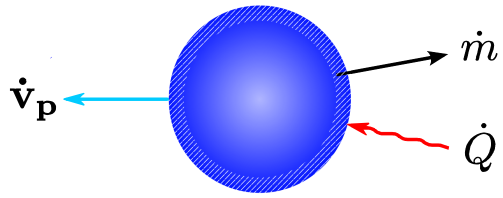


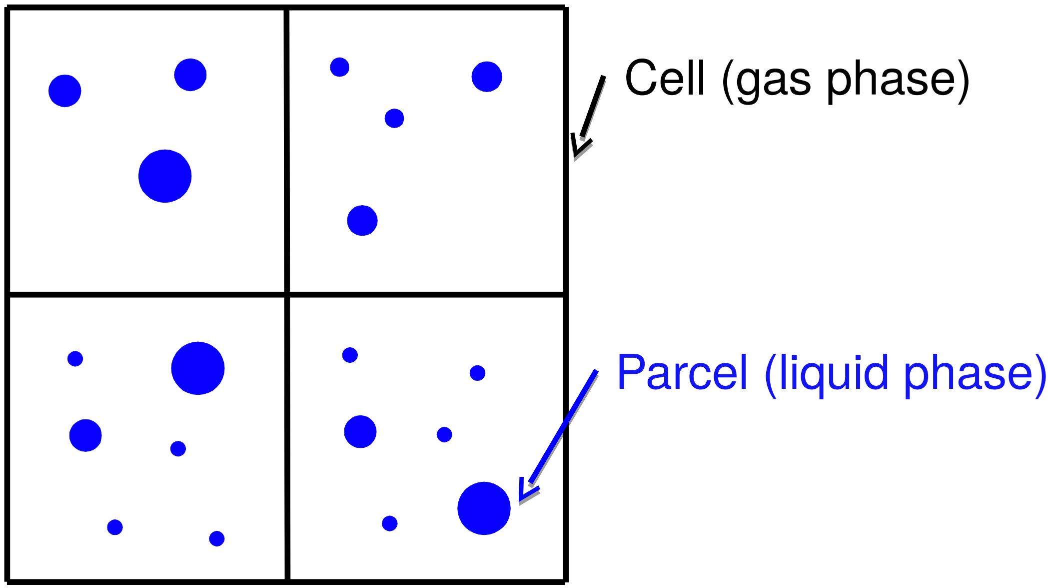
Lagrangian method

- Particle in cell method (PIC):
  - Statistical description
  - Follows evolution of parcels
  - Each parcel represents collection of identical droplets

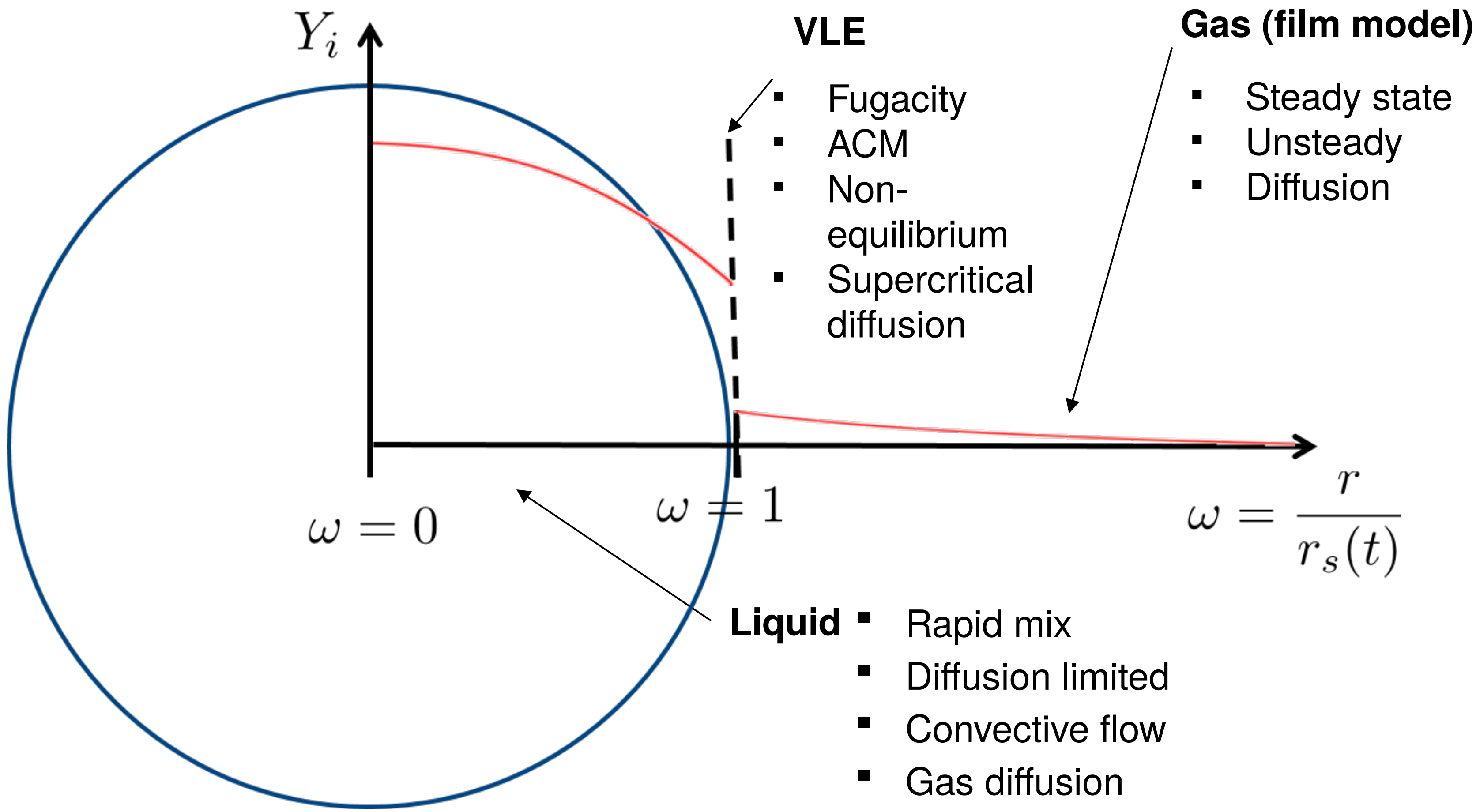
Gas-liquid coupling

- Momentum exchange
- Mass exchange
- Thermal exchange





Droplet modeling

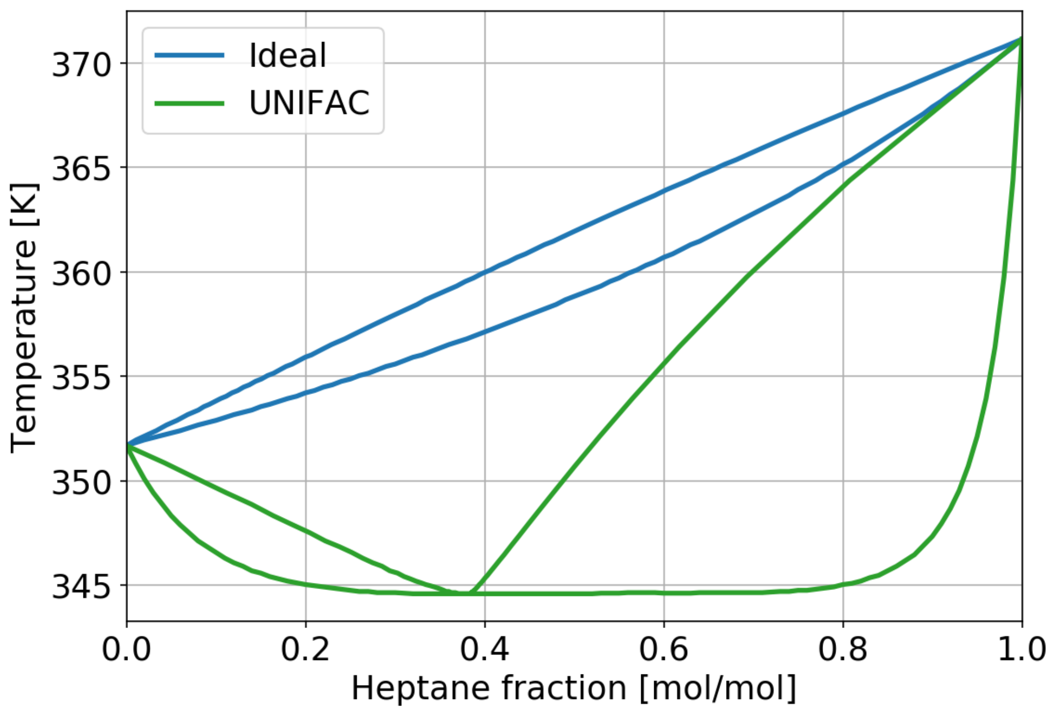


ULF

- Flexible framework for ODE/DAE system
- Run-time configurable and adaptable
- Coupling interface to external solver available
- Extended for solve single droplet evaporation with wide range of model

Vapor liquid equilibrium

VLE n-heptane/ethanol, 1 bar, UNIFAC vs ideal

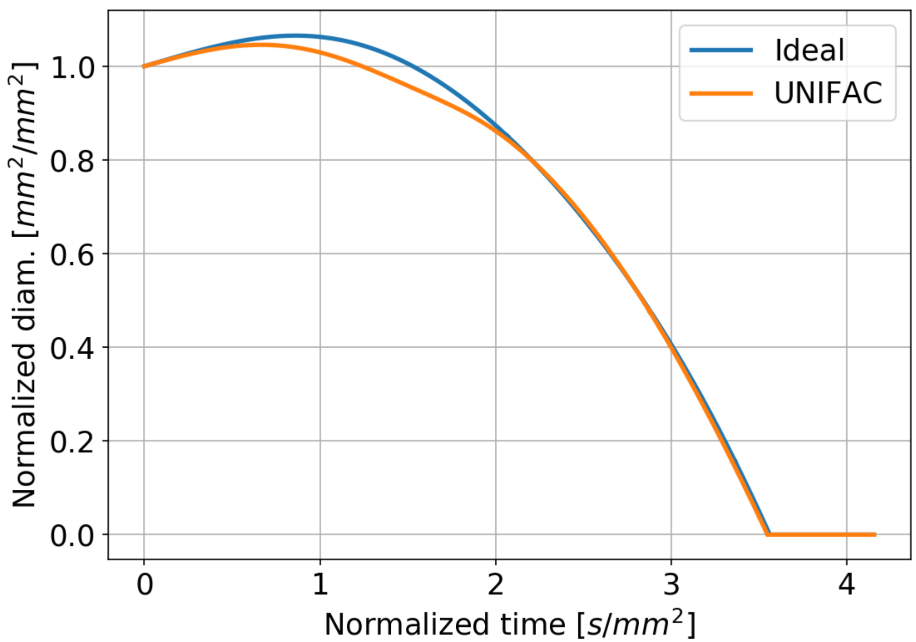


- Strong interacting species
  - Cannot be described with Raoult's law
  - Advanced model required (e.g. UNIFAC)
- Other models are run-time selectable
- Fugacity approach available

Single droplet

TECHNISCHE UNIVERSITÄT DARMSTADT

Ethanol/Heptane E10 (v/v), d_0 190 µm, T_{gas} 800 K, T_{liq} 320 K

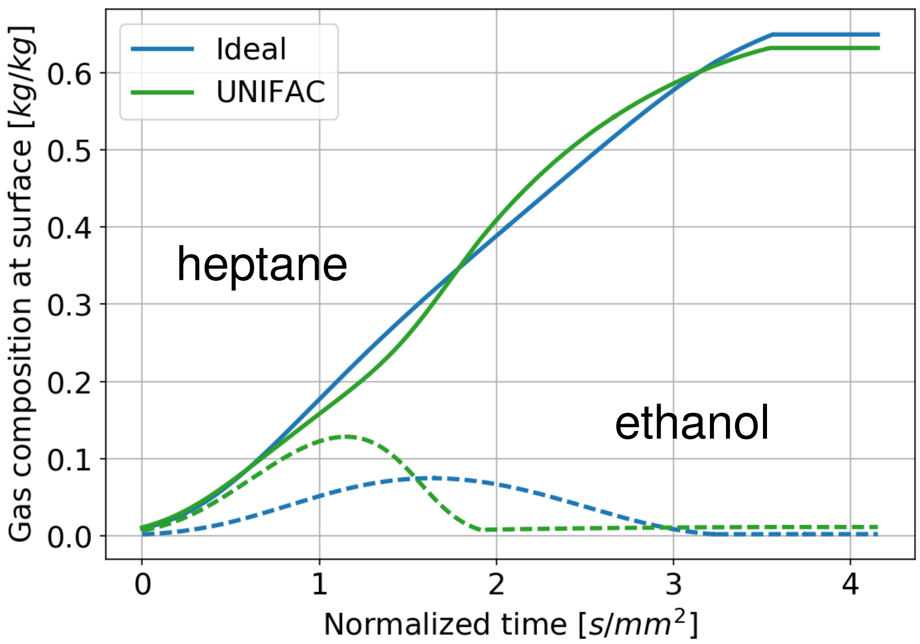


- Different VLE result in change in evaporation rate
- Effect is relevant in the transient evaporation phase

Single droplet

TECHNISCHE UNIVERSITÄT DARMSTADT

Ethanol/Heptane E10 (v/v), d_0 190 µm, T_{gas} 800 K, T_{liq} 320 K



- Gas composition at surface is affected by VLE

Single droplet

TECHNISCHE UNIVERSITÄT DARMSTADT

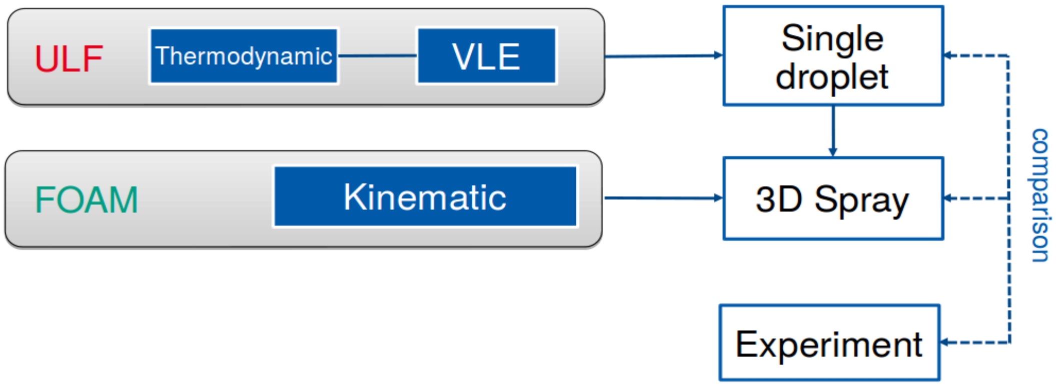
- Different models result in distinct droplet evolution
- Species interactions are important

↓

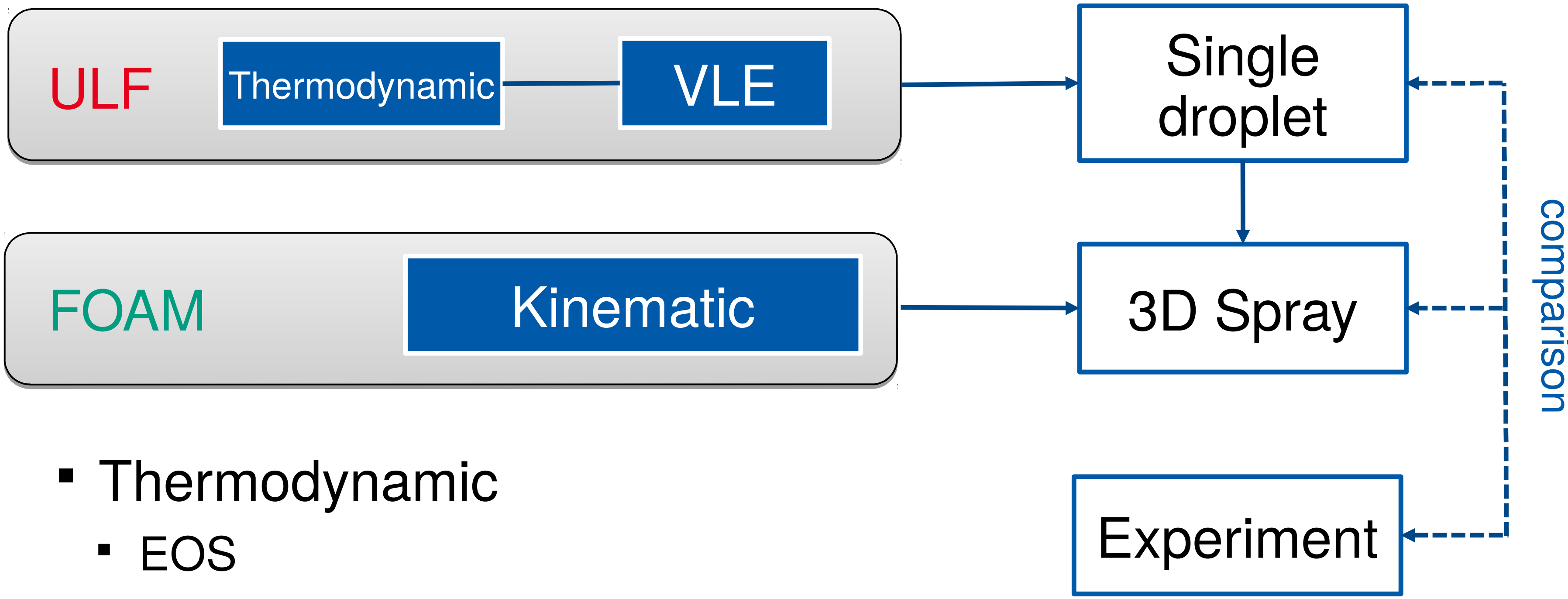
- Thermodynamical model direct affects:
  - Droplet evolution
  - Gas evolution
- Film properties around droplet are influenced by droplet model
- External droplet solver allows to study different model
- No modification in FOAM code necessary

Agenda

- Introduction
- ULF single droplet
- **Foam coupling**
- Validation
- Spray A
- Conclusion



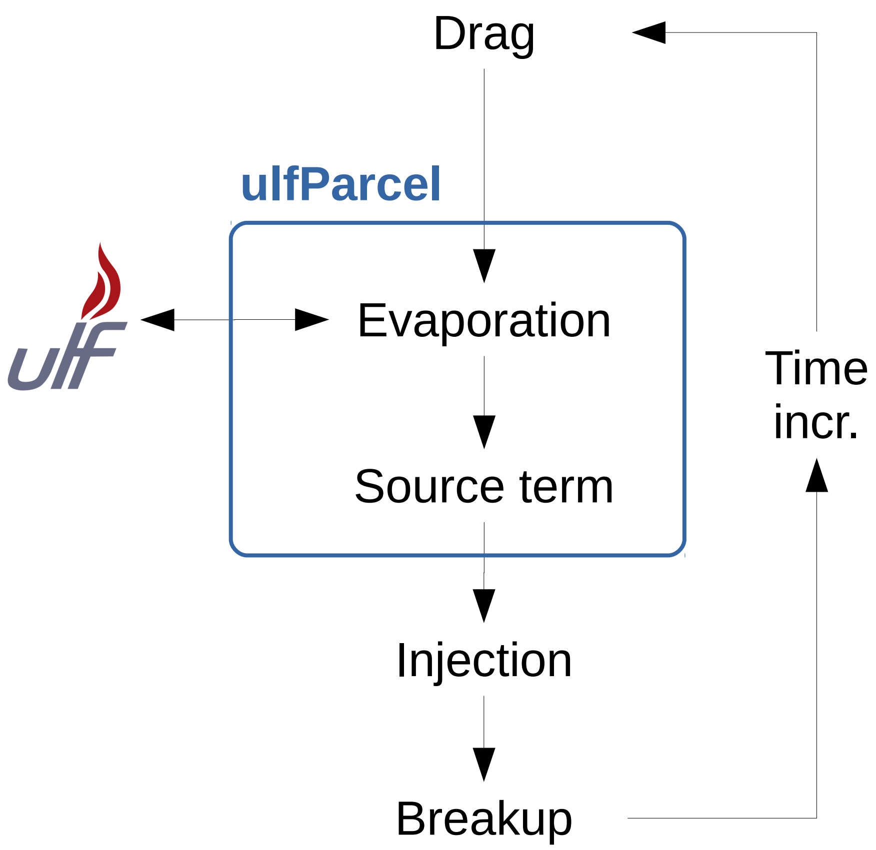
Coupling



- Thermodynamic
  - EOS
  - Fugacity
  - Activity coefficients
  - Heat capacity
  - ….

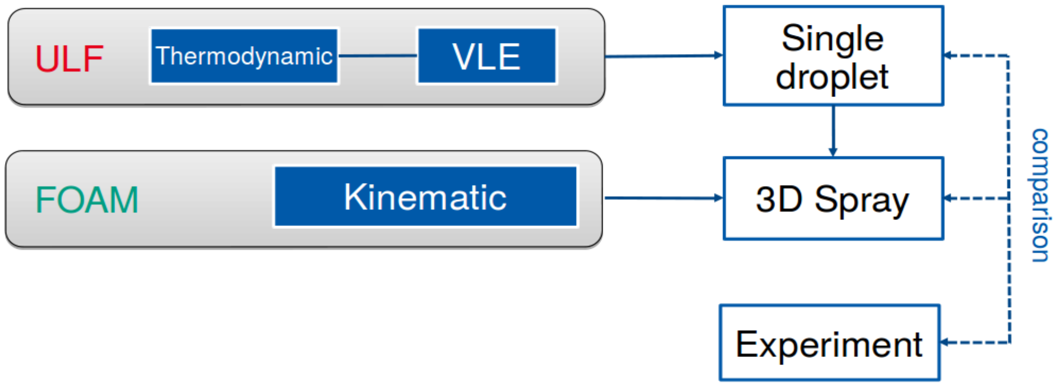
ulfParcel

- ulfParcel acts as interface with ULF
- It is responsible for:
  - Interact with foam Lagrangian tracking
  - Store info for breakup/collision/atom.
  - Interact with ULF to solve evaporation



Agenda

- Introduction
- ULF single droplet
- Foam coupling
- **Validation**
- Spray A
- Conclusion



Coupling

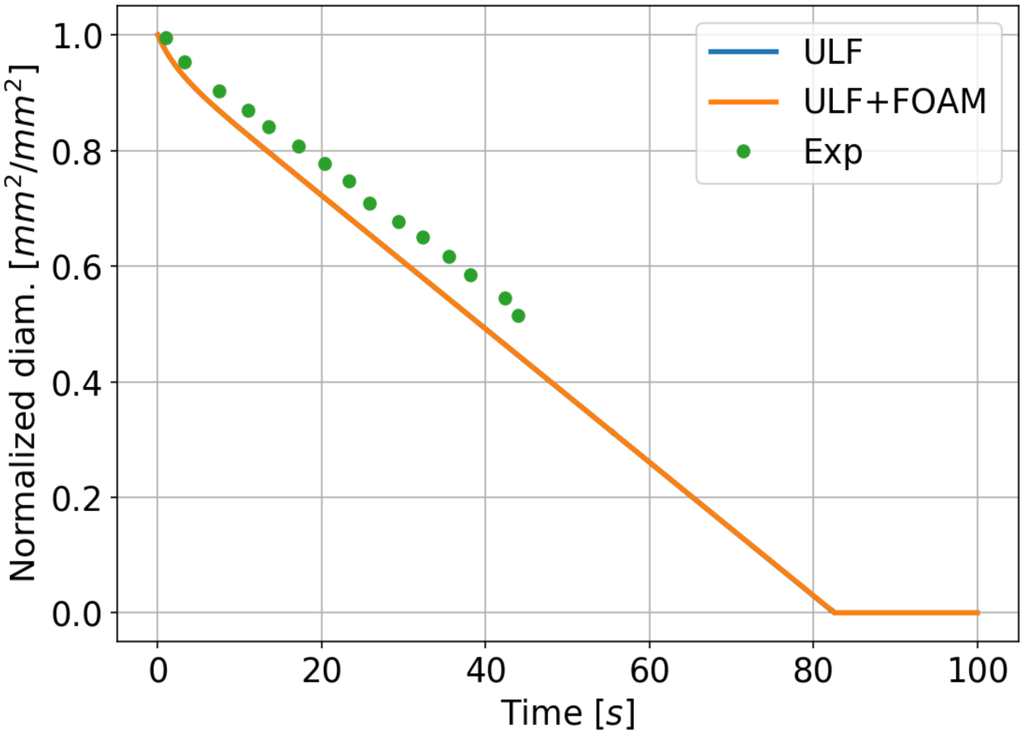
- Solution of the single droplet outsourced to a specialized solver (liquid, gas film, interface)
- OpenFOAM framework tracks the droplet parcel
  - Injection
  - Breakup
  - Drag
- High flexibility in solution

VALIDATION REQUIRED

- Single droplet
- Mass conservation
- Enthalpy conservation

Single droplet

Heptane, d_0 1180 µm, T_{gas} 297 K, T_{liq} 290 K, quiescent env.



- Verification against stand-alone and exp.

→ Evaporation rate correct

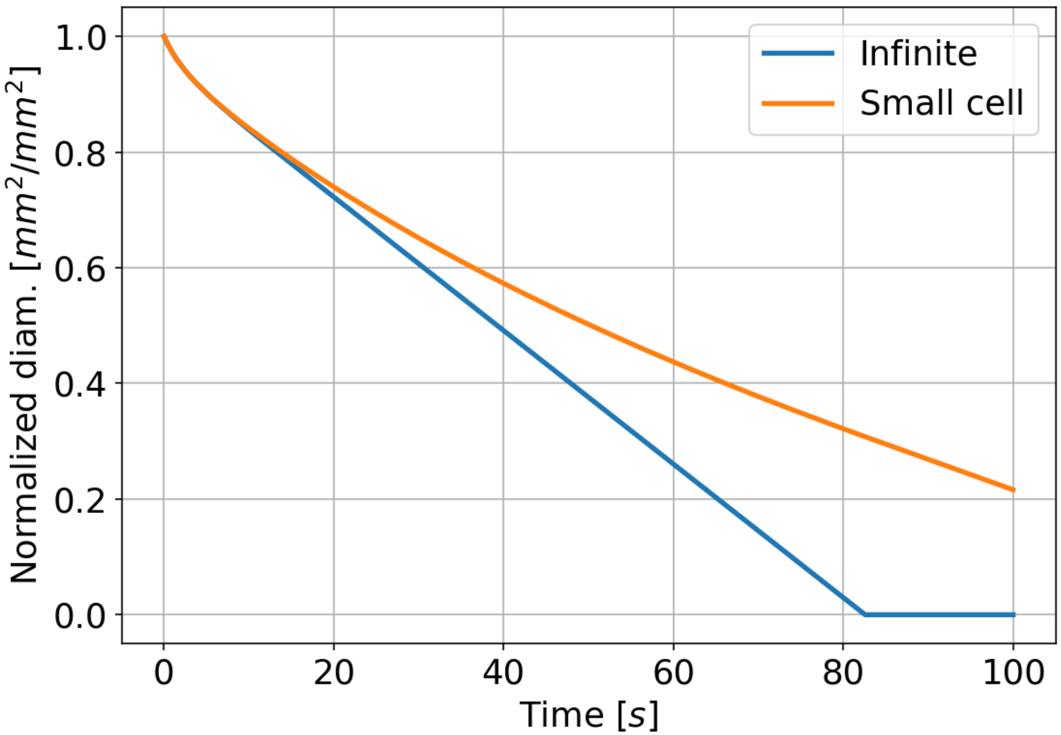
- One-way coupling correct
  - From ULF to FOAM

[1] Daif et al. Experimental Thermal and Fluid Science 18 (1999) 282-290

Single droplet

TECHNISCHE UNIVERSITÄT DARMSTADT

Heptane, d_0 1180 µm, T_{gas} 297 K, T_{liq} 290 K, quiescent env.

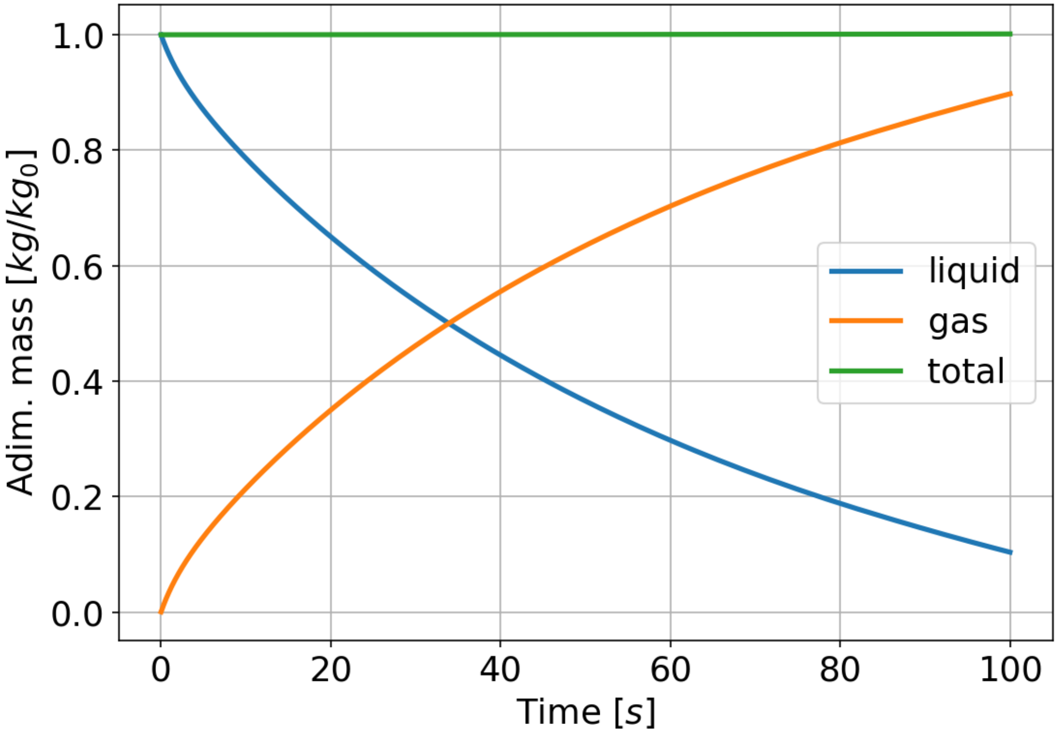


- Comparison with closed environment
  - 10x10x10 mm
- Saturation slows down evaporation rate
- Two-way coupling correct

Mass conservation

TECHNISCHE UNIVERSITÄT DARMSTADT

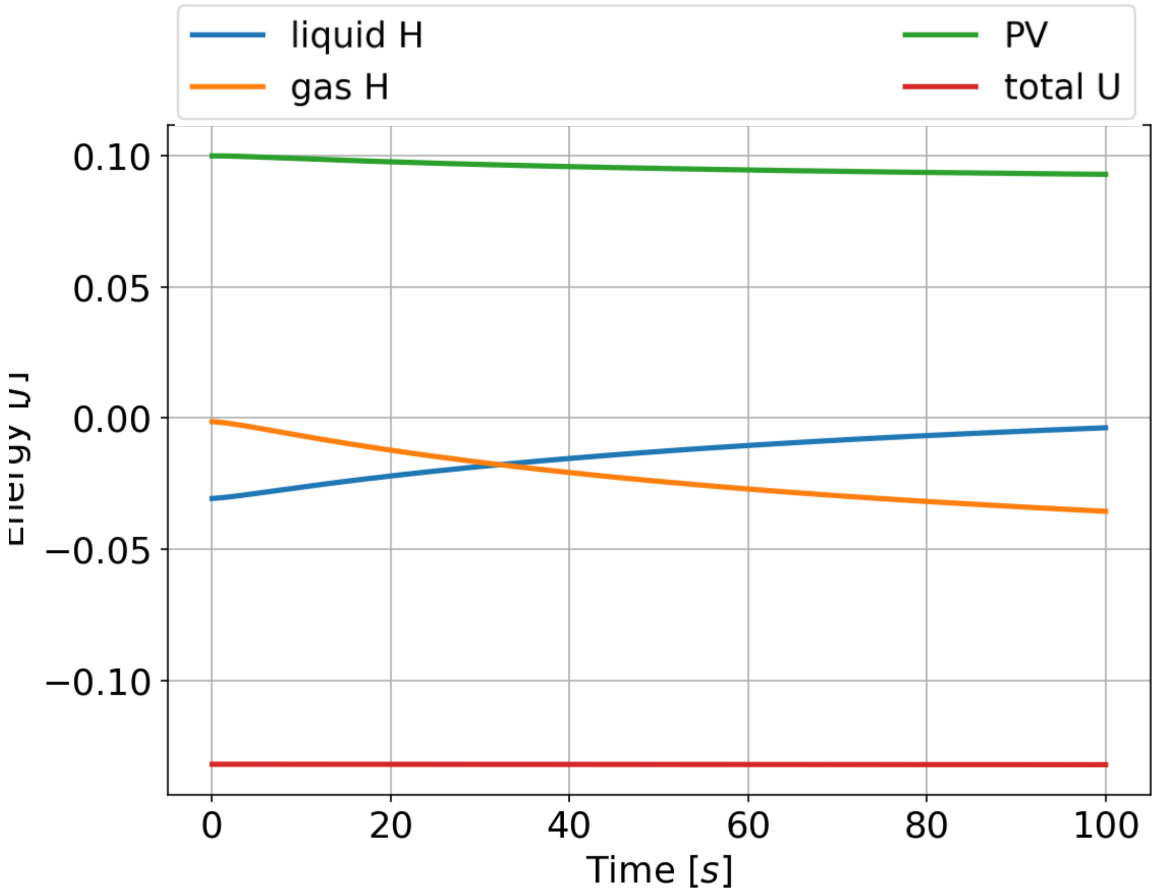
Heptane, d_0 1180 µm, T_{gas} 297 K, T_{liq} 290 K, quiescent env.



- Closed system
- Mass conserved

Energy conservation

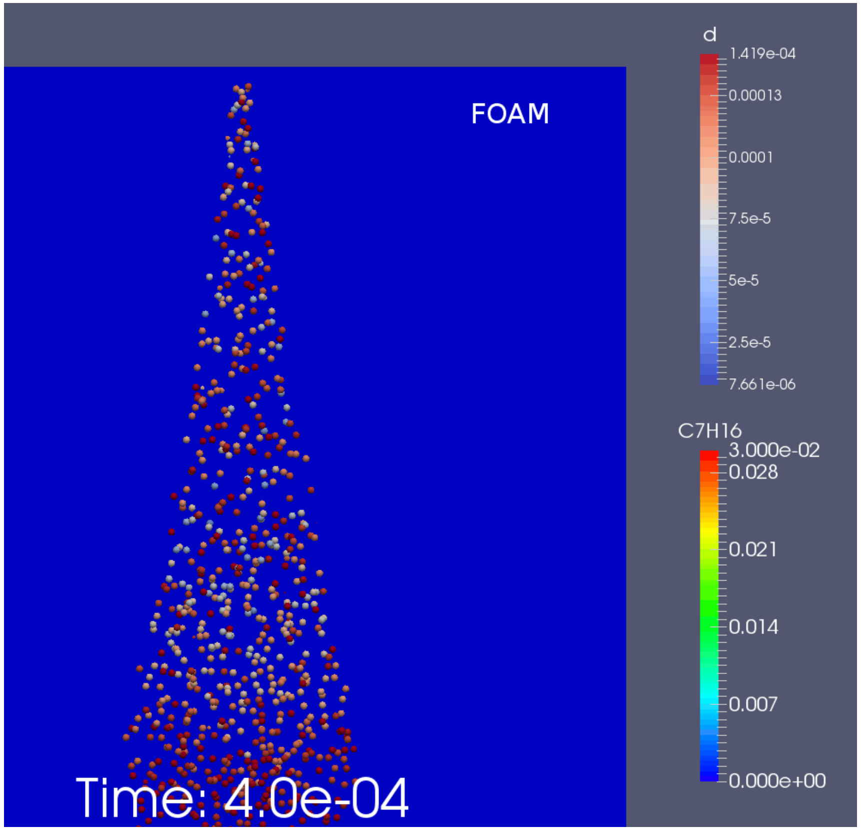
Heptane, d_0 1180 µm, T_{gas} 297 K, T_{liq} 290 K, quiescent env.



- Closed system
- Energy conserved
- Drop in pressure due to cooling down

Lagrangian tracking

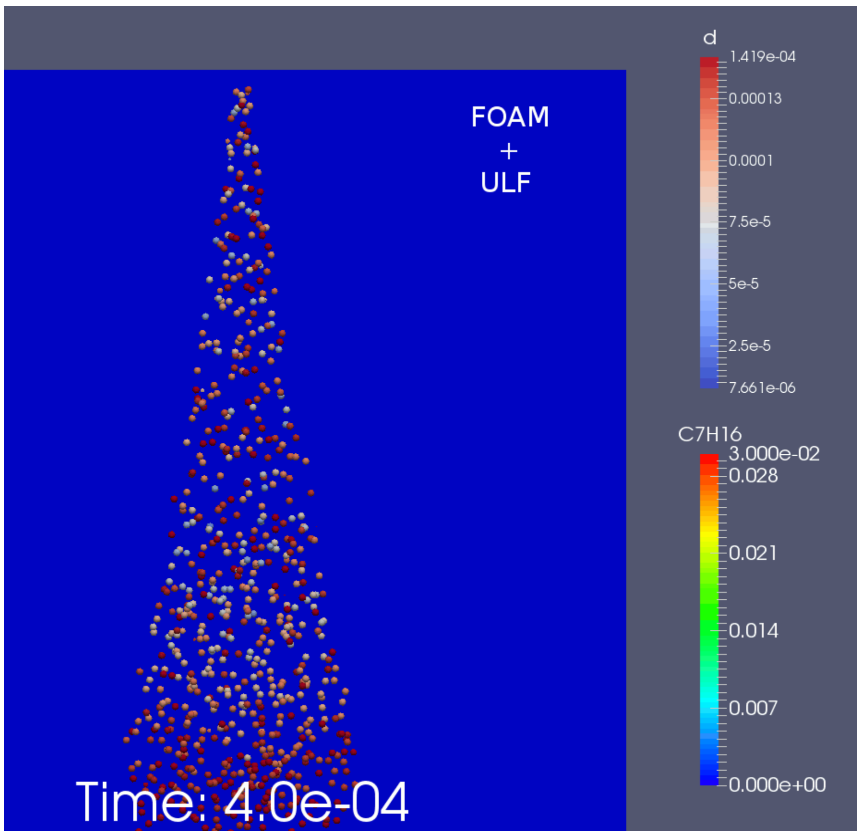
Heptane, aachenBomb Case, T_{gas} 800 K, T_{liq} 320 K, p 5 MPa



- Nitrogen environment
  - No combustion
- Only injection and drag
- Coupling does not affect lagrangian tracking
- Injection properties transferred to ulfParcel

Lagrangian tracking

Heptane, aachenBomb Case, T_{gas} 800 K, T_{liq} 320 K, p 5 MPa

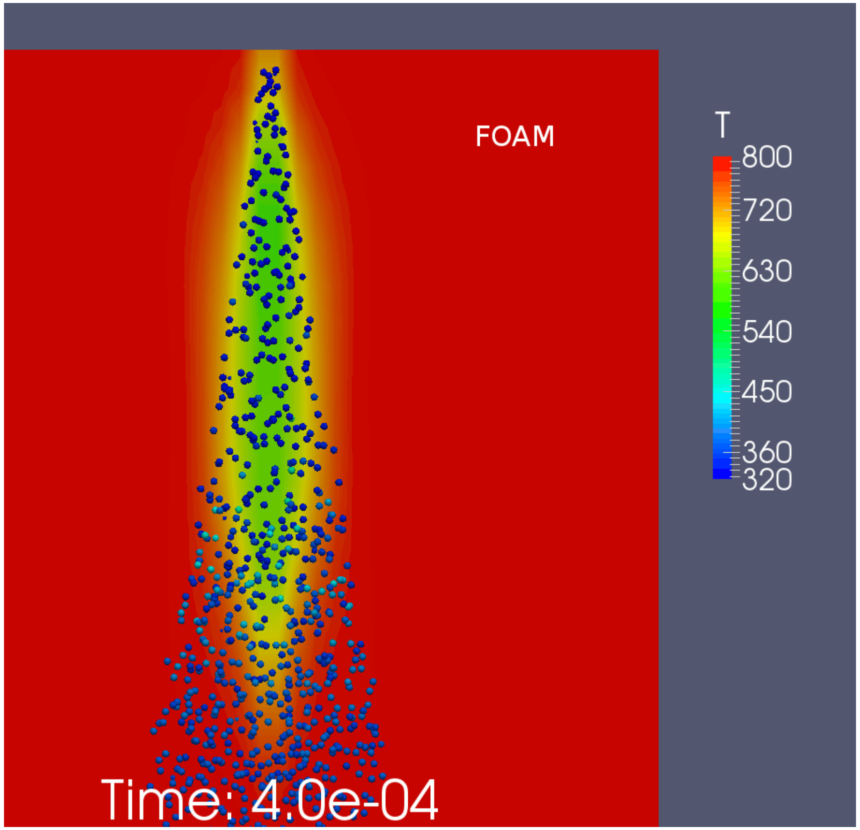


- Nitrogen environment
  - No combustion
- Only injection and drag
- Coupling does not affect lagrangian tracking
- Injection properties transferred to ulfParcel

Heat transfer

TECHNISCHE UNIVERSITÄT DARMSTADT

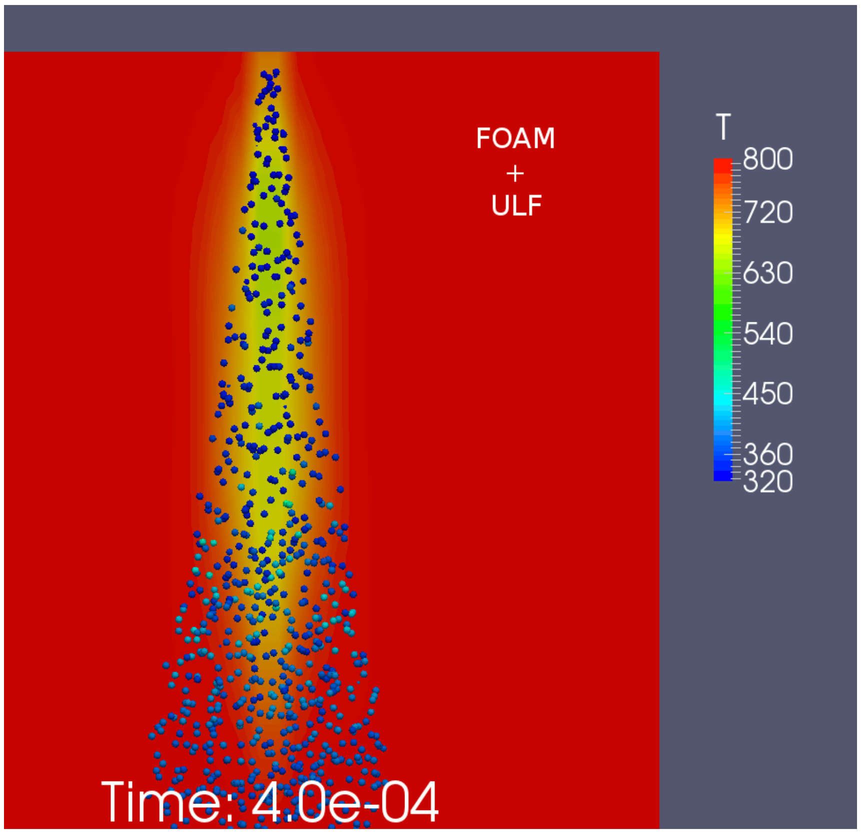
Heptane, aachenBomb Case, T_{gas} 800 K, T_{liq} 320 K, p 5 MPa



- Only heat transfer
- Spray morphology is unchanged
- Temperature field slight different
  - → Minor thermal exchange for FOAM+ULF solver

Heat transfer

Heptane, aachenBomb Case, T_{gas} 800 K, T_{liq} 320 K, p 5 MPa



- Only heat transfer
- Spray morphology is unchanged
- Temperature field slight different
  - → Minor thermal exchange for FOAM+ULF solver

Validation of 3D spray

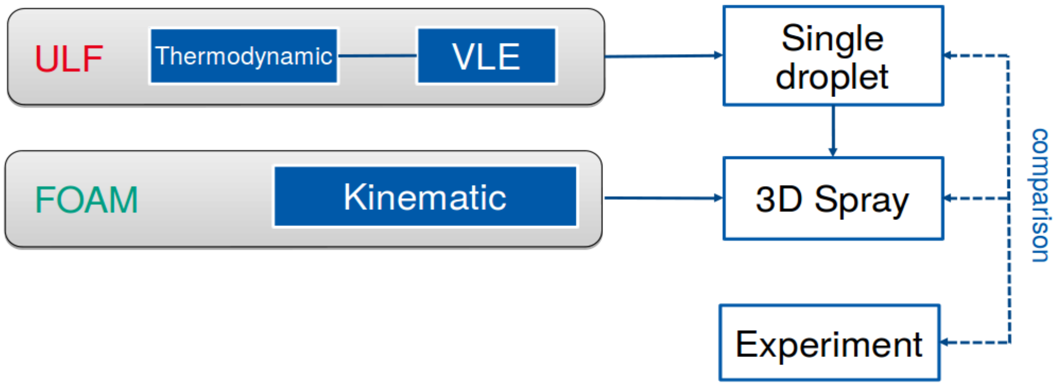
- The coupling does not affect the spray
- Lagrangian tracking is correct
- Thermal transfer are comparable

↓

Coupling is a suitable technique for spray modelling

Agenda

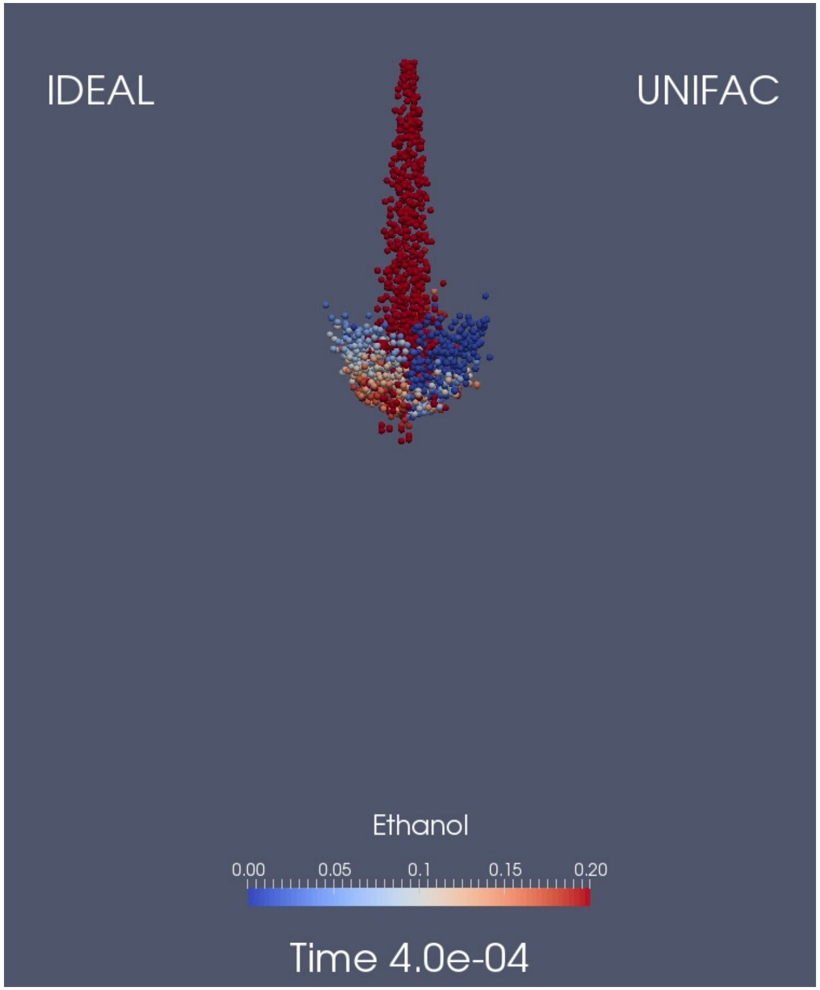
- Introduction
- Single droplet
- Foam coupling
- Validation
- **Spray A**
- Conclusion



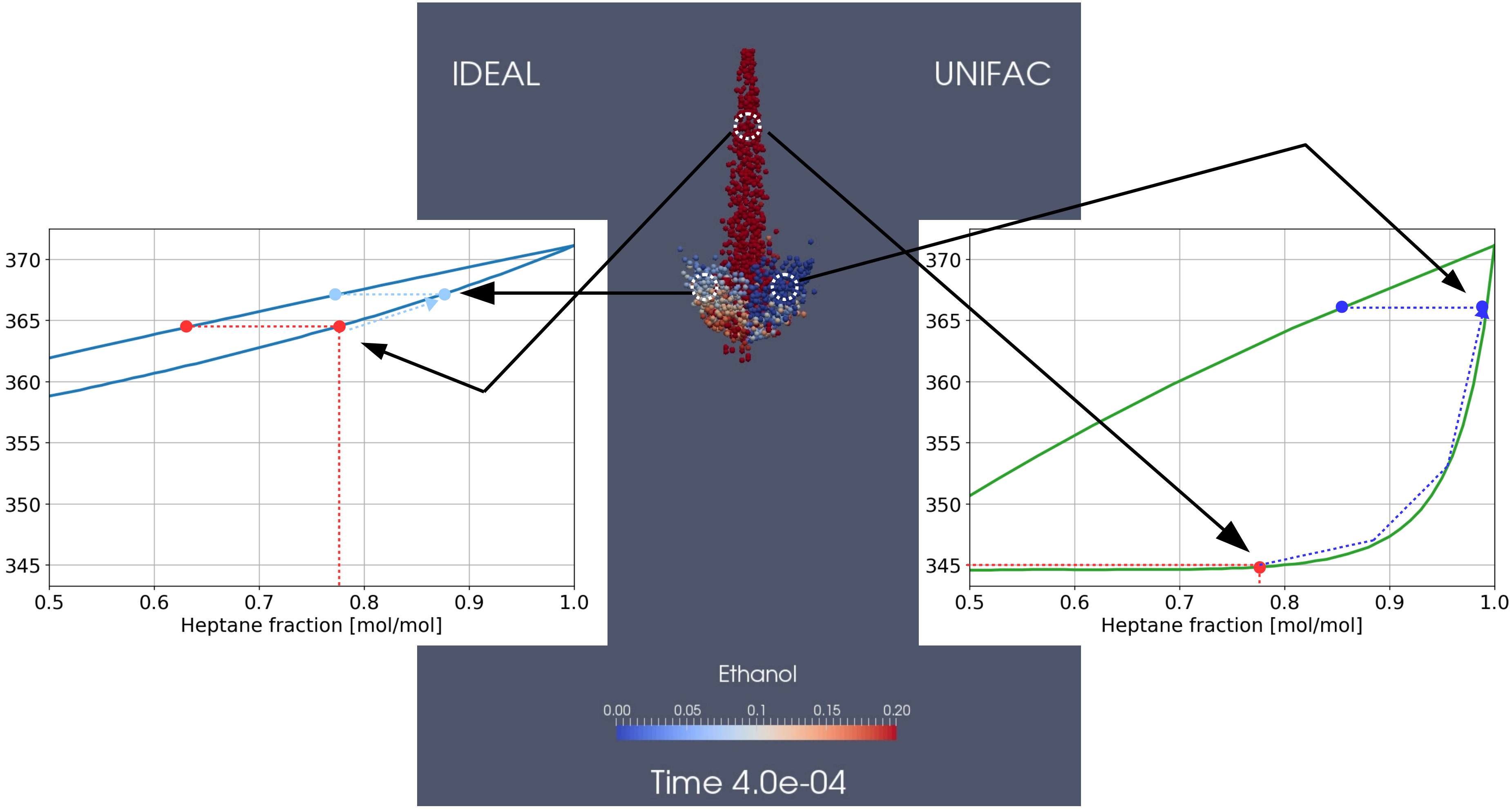
Spray A

- Next slides will show some possibilities of this method in describe spray of complex mixture
- AachenBomb
  - ReitzKHRT
  - Cone injection
  - Heptane 90%, ethanol 10% (vol/vol)
  - Mass evaporation

Spray A



Spray A


IDEAL
UNIFAC
370
365
360
355
350
345
0.5
0.6
0.7
0.8
0.9
1.0
Heptane fraction [mol/mol]
Ethanol
0.00
0.05
0.1
0.15
0.20
Time 4.0e-04

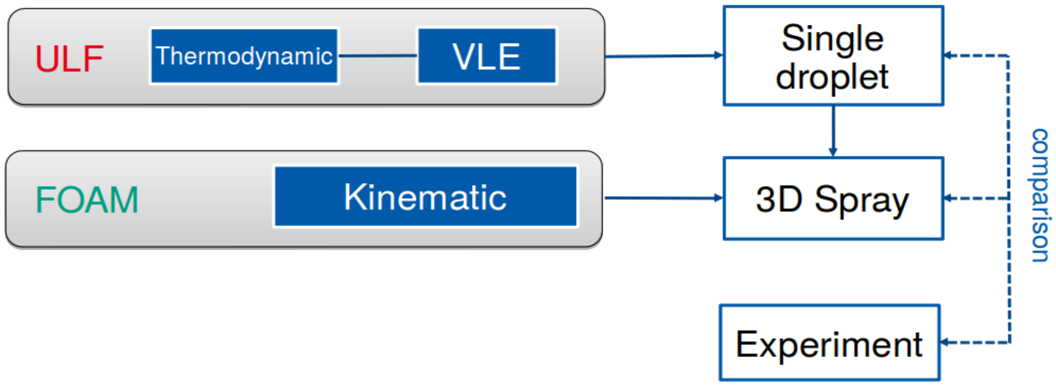
Spray A

- Droplet evolution affected by interface thermodynamic

- Properly choose of the model is crucial for a proper spray simulation
- Run time selection of droplet model is important

Agenda

- Introduction
- ULF single droplet
- Foam coupling
- Validation
- Spray A
- **Conclusion**



Conclusion

- A new method to solve lagrangian spray is introduced
- The parcel is an interface to an external specific solver for single droplet evaporation
- External solver run-time selects different model
  - Liquid
  - VLE
  - Gas film
- Foam manages injection, breakup and tracking
- Conservation of quantities is verified for single droplet
- 3D spray tracking is not affected by the external solver
- Biofuel spray evolution with different model are shown