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

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

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Agenda

- 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)

Droplet modeling

\[ \omega = 0 \quad \omega = 1 \quad \omega = \frac{r}{r_s(t)} \]

Liquid

VLE

Gas
Droplet modeling

VLE
- Fugacity
- ACM
- Non-equilibrium

Gas
- Steady state
- Unsteady
- Diffusion approach

Liquid
- Rapid mix
- Diffusion limited
- Convective flow
- Gas diffusion

\[ \omega = 0 \quad \omega = 1 \quad \omega = \frac{r}{r_s(t)} \]
Droplet modeling

\[ Y_i \]

\[ \omega = 0 \quad \omega = 1 \]

VLE

- Fugacity
- ACM
- Non-equilibrium
- Supercritical diffusion

\[ Y_i = \frac{\gamma_i X_i f_i^0}{\varphi_i \rho} = \frac{X_i p_i^0 \gamma_i \varphi_i^0}{\rho \varphi_i} \mathrm{Poy}_i \]
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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

Cell (gas phase)
Parcel (liquid phase)
Droplet modeling

VLE
- Fugacity
- ACM
- Non-equilibrium
- Supercritical diffusion

Gas (film model)
- Steady state
- Unsteady
- Diffusion

Liquid
- Rapid mix
- Diffusion limited
- Convective flow
- Gas diffusion
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

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

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

Ethanol/Heptane E10 (v/v), \( d_0 \) 190 \( \mu \text{m} \), \( T_{\text{gas}} \) 800 K, \( T_{\text{liq}} \) 320 K

- Gas composition at surface is affected by VLE
Single droplet

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

- Thermodynamical model directly affects:
  - Droplet evolution
  - Gas evolution

- Film properties around droplet are influenced by droplet model
- External droplet solver allows to study different models
- No modification in FOAM code necessary
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Coupling

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

ULF Thermodynamic VLE

FOAM Kinematic

Single droplet
3D Spray
Experiment

Comparison
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
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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, $T_{\text{gas}}$ 297 K, $T_{\text{liq}}$ 290 K, quiescent env.

- Verification against stand-alone and exp.
- Evaporation rate correct
- One-way coupling correct
  - From ULF to FOAM

Single droplet

Heptane, $d_0 = 1180 \, \mu m$, $T_{\text{gas}} = 297 \, K$, $T_{\text{liq}} = 290 \, K$, quiescent env.

- Comparison with closed environment
  - $10x10x10 \, mm$
- Saturation slows down evaporation rate
- Two-way coupling correct
Mass conservation

Heptane, $d_0 \, 1180 \, \mu m$, $T_{\text{gas}} \, 297 \, K$, $T_{\text{liq}} \, 290 \, K$, 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, $T_{\text{gas}} = 800$ K, $T_{\text{liq}} = 320$ 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, $T_{\text{gas}} = 800 \text{ K}$, $T_{\text{liq}} = 320 \text{ K}$, $p = 5 \text{ MPa}$

- Nitrogen environment
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Heat transfer

Heptane, aachenBomb Case, $T_{\text{gas}}$ 800 K, $T_{\text{liq}}$ 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, $T_{\text{gas}} = 800 \text{ K, } T_{\text{liq}} = 320 \text{ K, p } 5 \text{ MPa}$

- Only heat transfer
- Spray morphology is unchanged
- Temperature field slight different

$\rightarrow$ 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
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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

Heptane fraction [mol/mol]

Ethanol

Time 4.0e-04

Heptane fraction [mol/mol]
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
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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