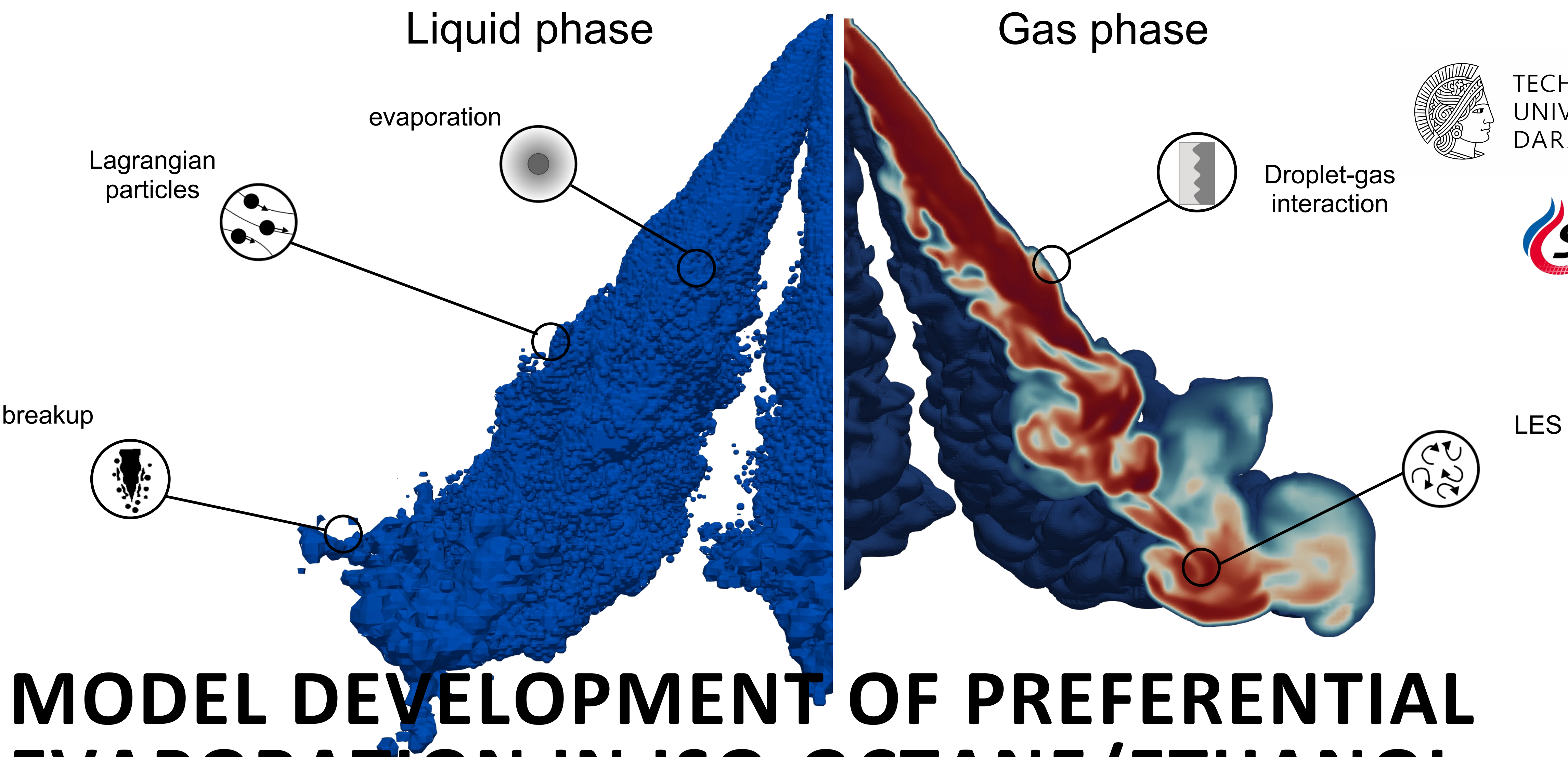
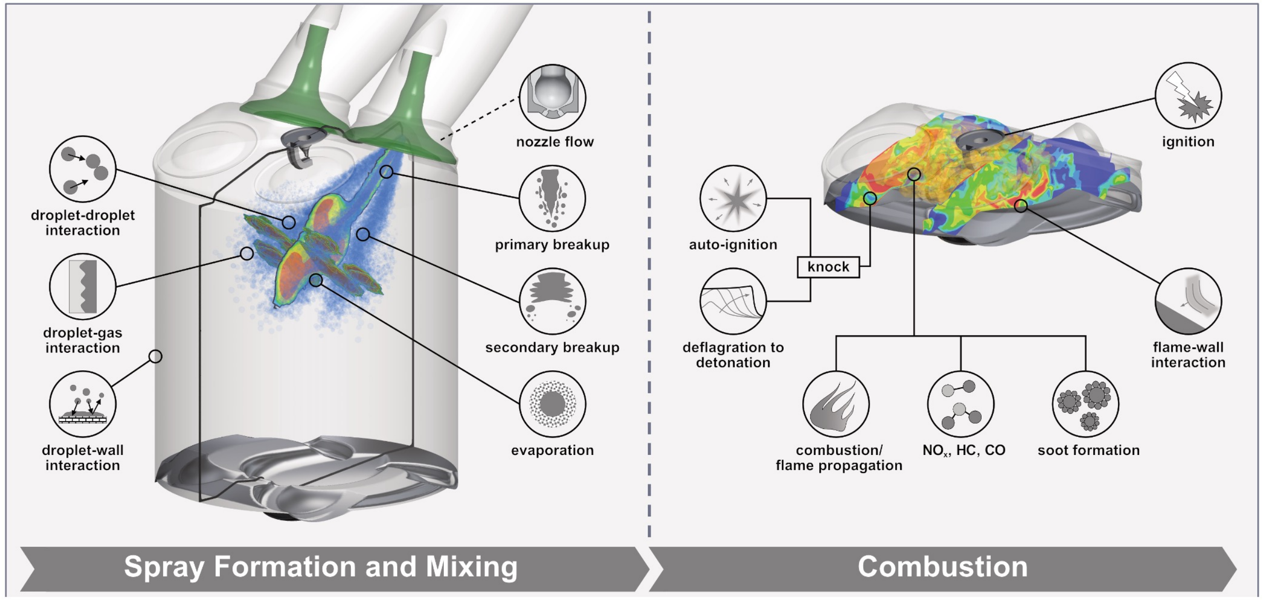


MODEL DEVELOPMENT OF PREFERENTIAL EVAPORATION IN ISO-OCTANE/ETHANOL SPRAYS

MOTIVATION



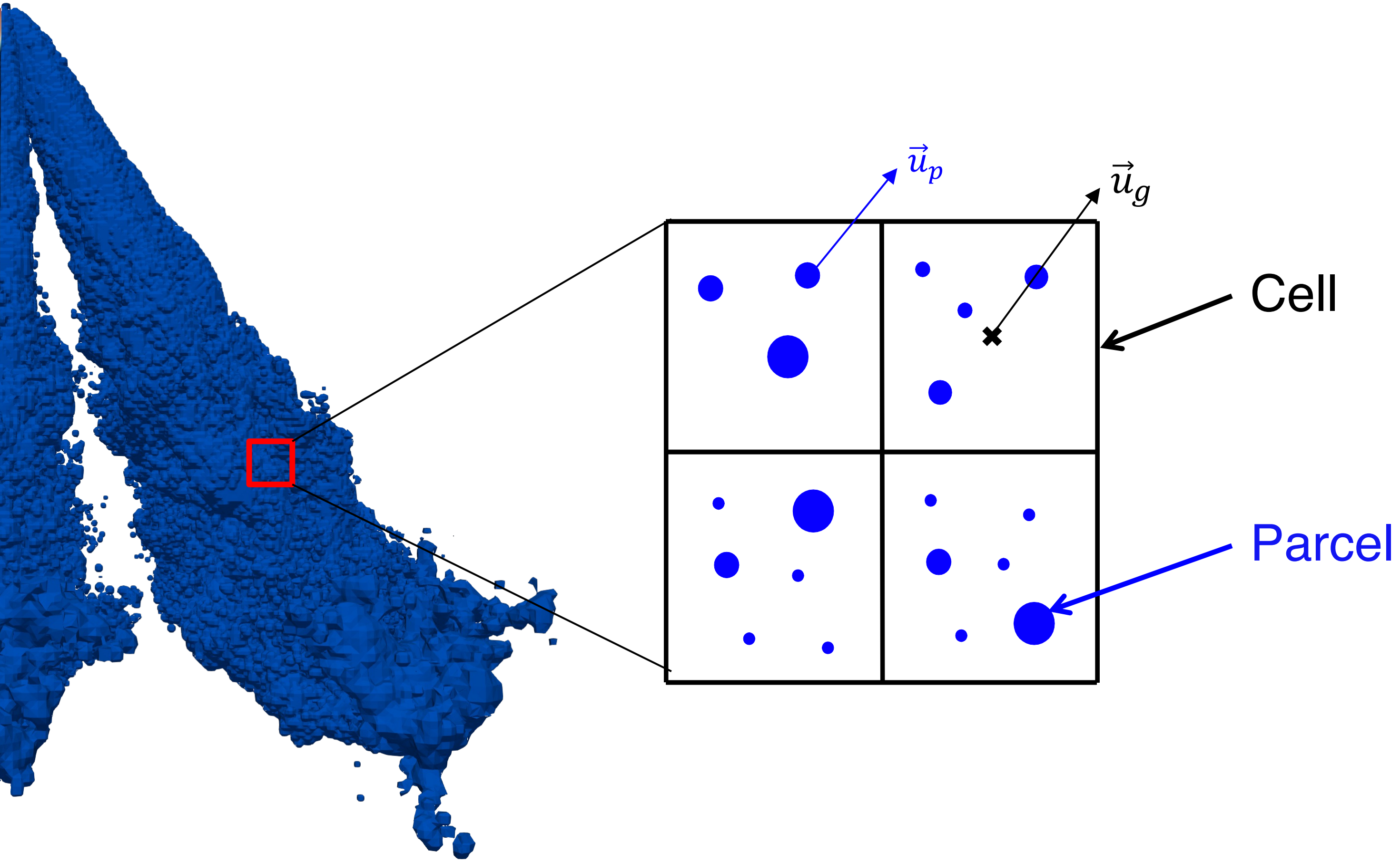
Requirements of modern combustion engines:

- Low pollutant emission
- Move towards CO_2 neutral fuels
  - Ethanol as promising renewable fuel
- Combustion efficiency

New Challenges:

- Different spray & mixture formation
- Combustion phase cannot be looked at independently (motor-effect chain)

SPRAY MODELING



Particle in cell method/ Euler Lagrange method

- Statistical description
- Follows evolution of parcels
- Each parcel represents collection of identical droplets

PARTICLE MODELING

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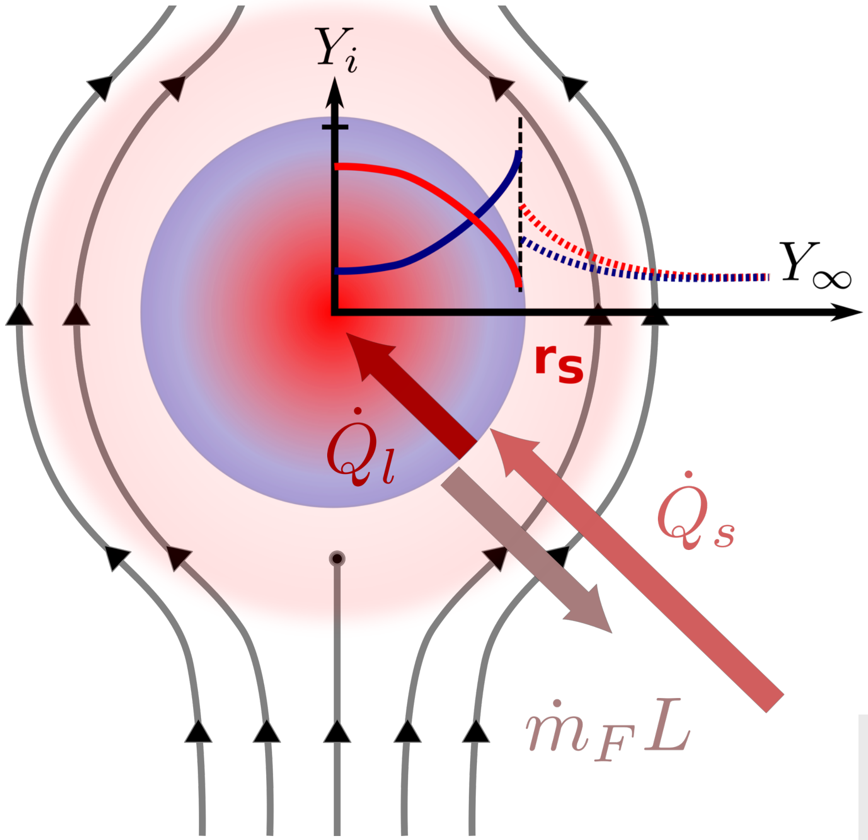


Transport processes:

- Momentum
- Temperature
- Species

$$\frac{d\,u_p}{dt} = \frac{3}{4} \mathrm{C_D Re}_p \frac{\mu_g}{\rho_p d^2} u_{rel} + g$$

$$\frac{dT_p}{dt} = \frac{\dot{Q}_s - \dot{m}_F L}{m_d c_{p,l}}$$

Interface modeling

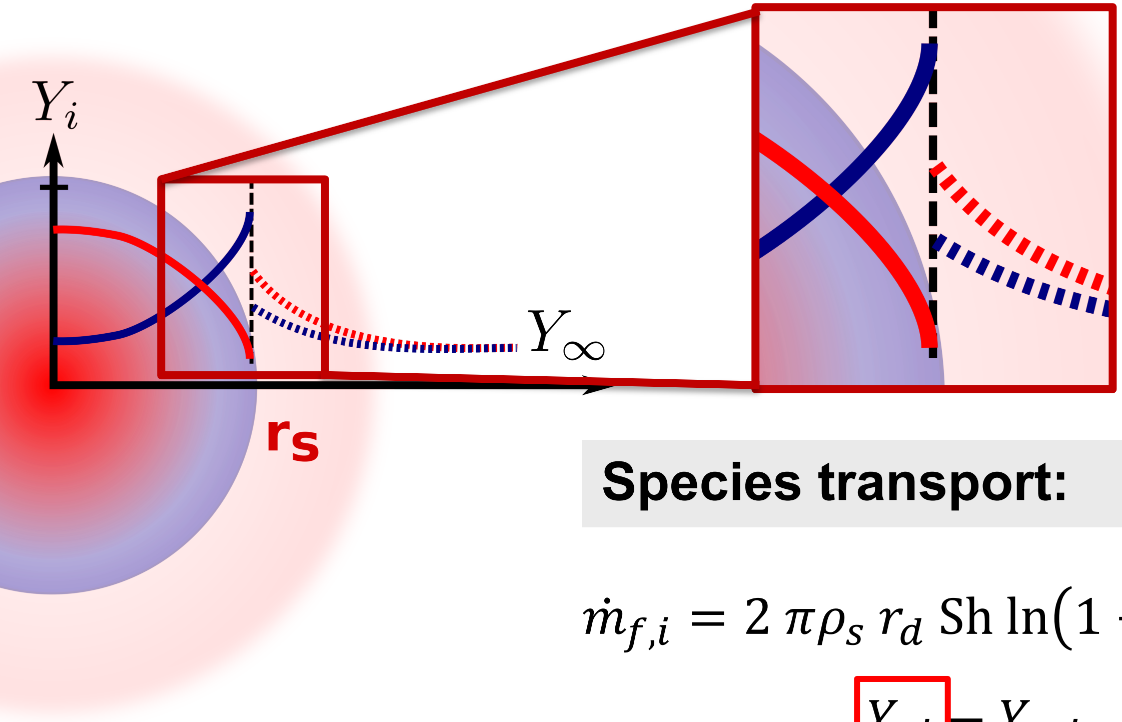
- Vapor liquid equilibrium (VLE)
- preferential evaporation
- Usually ideal liquid and gas

Heat transfer

- Convective heat transfer

$$\dot{Q}_s = \pi d_p k_g \mathrm{Nu}\,(T_\infty - T_s)$$

EVAPORATION MODELING



Species transport:

$$\dot{m}_{f,i} = 2\,\pi \rho_s\, r_d\, \mathrm{Sh}\, \ln\left(1 + B_{m,i}\right)$$

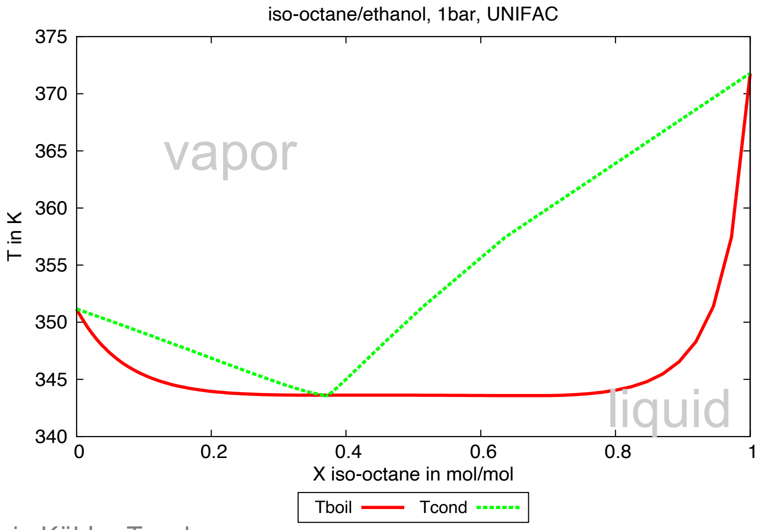
$$B_{m,i} = \frac{Y_{s,i} - Y_{\infty,i}}{1 - Y_{s,i}}$$

Ideal (Raoult's law) :

$$X_{s,i} = X_{l,i}\,\frac{p_{vap,i}}{p}$$

Real :

- ACMs (e.g. UNIFAC)
- Tabulation



REAL THERMODYNAMIC MODELING

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Real VLE :

$$f_i^v(p,T,x_i^v) = f_i^l(p,T,x_i^l)$$

$\Phi - \gamma$ approach:

$$\varphi_i^v X_i^v p = \gamma_i^l X_i^l f_j^{l,0}$$

fugacity coefficient (φ_i^v)

activity coefficient (γ_i^l)

reference fugacity ($f_j^{l,0}$)

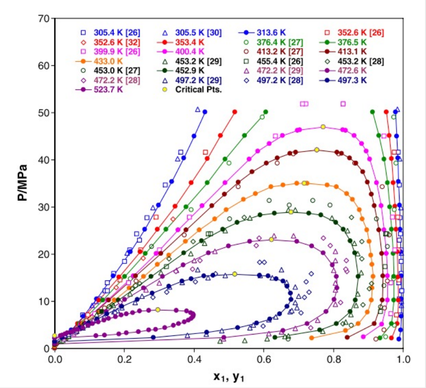
$$X_i^v p = \gamma_i^l X_i^l p_i^{sat}$$

UNIFAC:

$$\gamma_i^l = f(T, X_i^l, X_j^l)$$

Tabulation :

- Obtain VLE Data:



- Generate Table

Input		Output
p_{VLE}	T_{VLE}	$Y_{i,gas}$

- Look up during runtime

$$X_{s,i} = f(p_{cell}, T_p)$$

APPROACH

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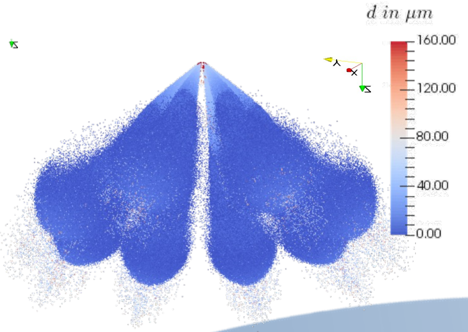

single droplet

droplet chain

spray

complexity

validation

experiments

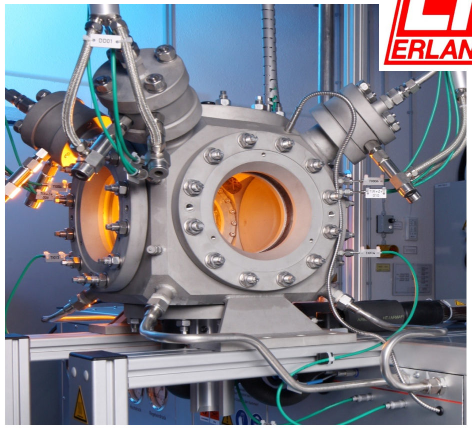

Image Source: LTT-FAU Erlangen

SINGLE DROPLET MODELING

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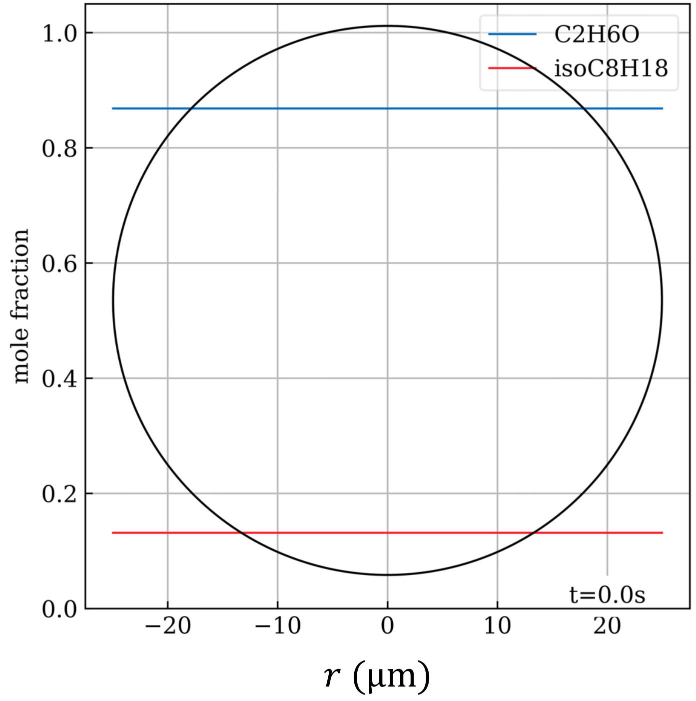
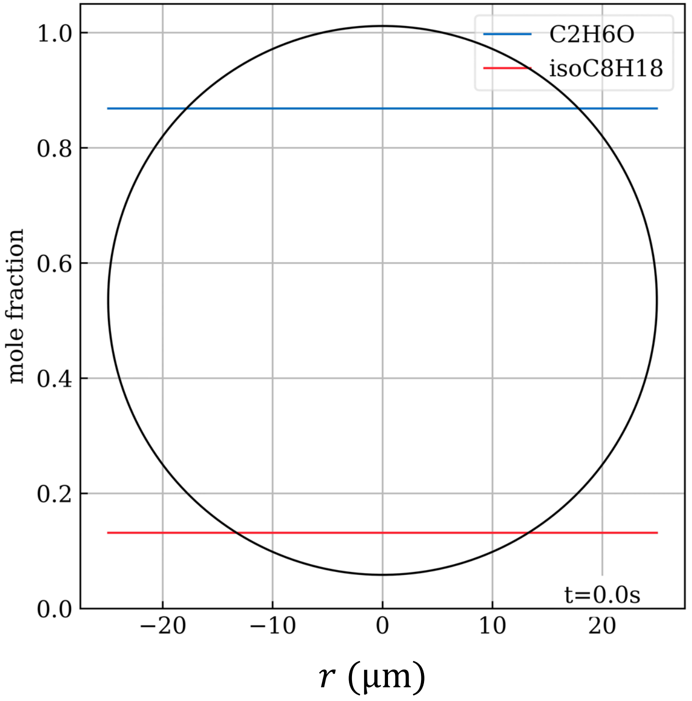
ideal (Raoult's law)



real VLE (UNIFAC)



boundary conditions

$T_U = 297$ K

$T_d = 333\ K$

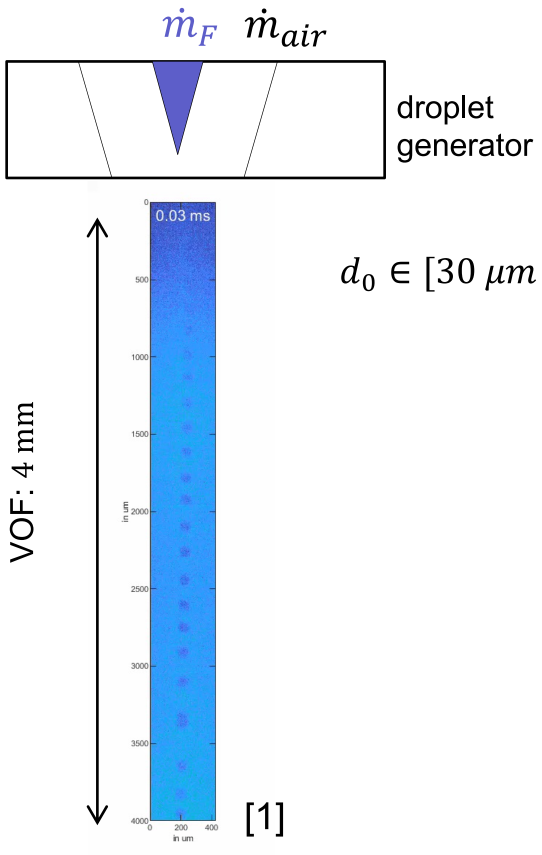
$d_0 = 50\ \mu m$

$v_0 = 7\ \frac{m}{s}$

vol% = e70

- Ideal model doesn't capture ethanol accumulation in e70 drop
- Different mixture formation depending on the initial ethanol concentration

DROPLET CHAIN



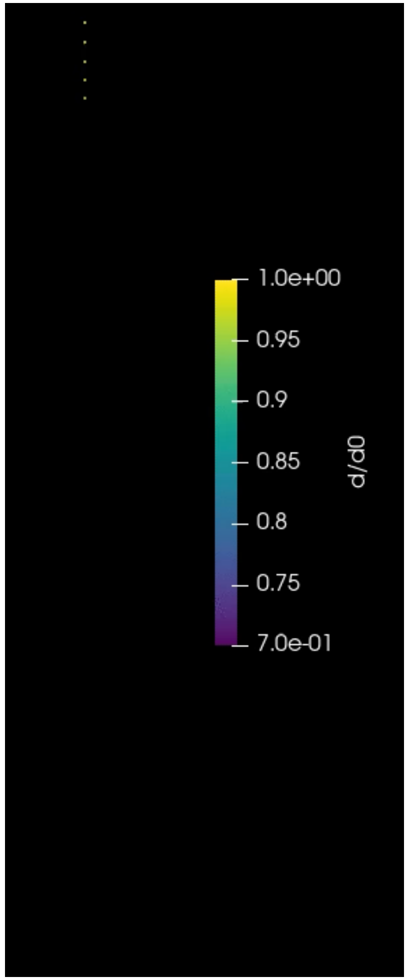
$d_0 \in [30\ \mu m\ ; 100\ \mu m]$

Experiment:

- Measurement of
  - Droplet diameter
  - Iso-octane/ethanol ratio in droplet
- Variation of droplet diameter & initial droplet temperature, fuel composition

- Variation of ambient temperature

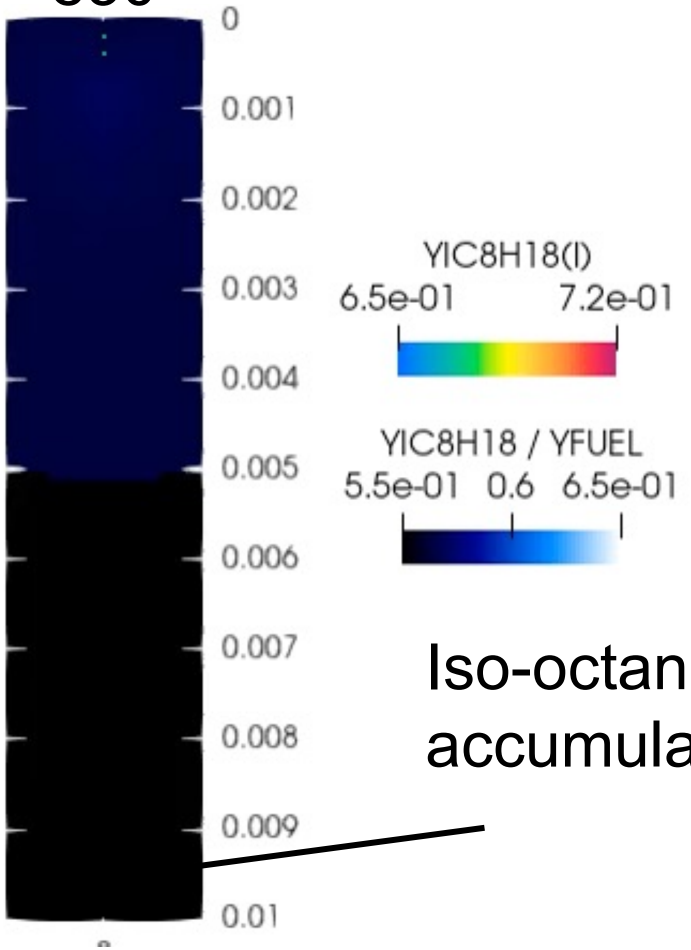
Simulation:



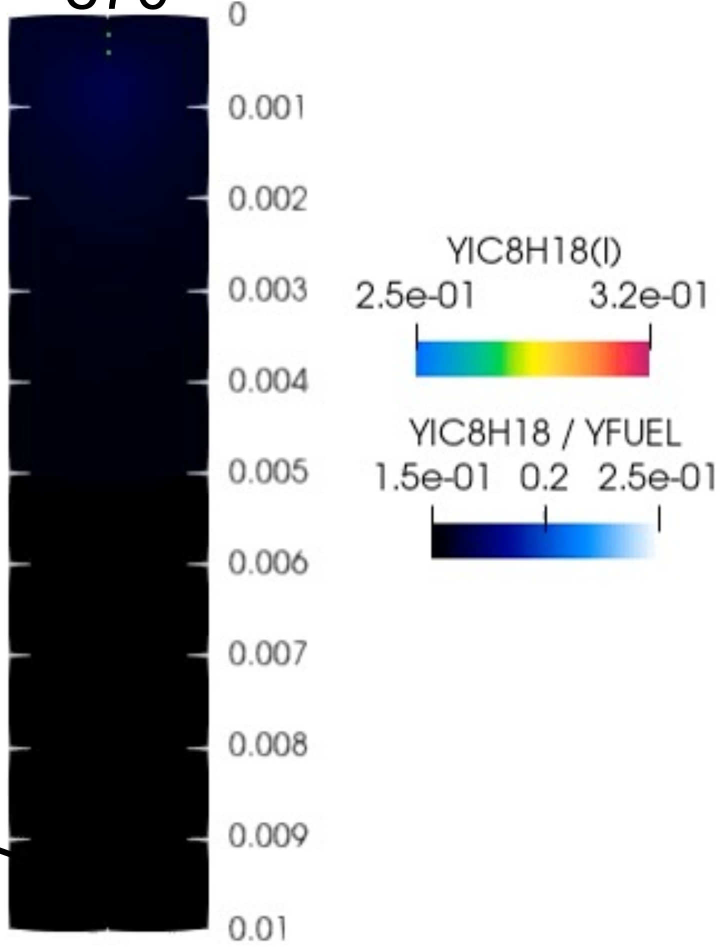
[1] video provided by LTT FAU Erlangen

IDEAL DROPLET CHAIN

e30

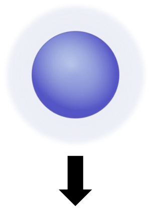


e70



Iso-octane accumulation in droplet

boundary conditions



$T_U = 547\ \mathrm{K}$

$T_d = 333\ K$

$d_0 = 70\ \mu m$

$v_0 = 7\ \frac{m}{s}$

$\mathbf{vol\% = e30, e70}$

- With real VLE different mixture formation expected

SPRAY – EXPERIMENTAL DATA

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G1 conditions:

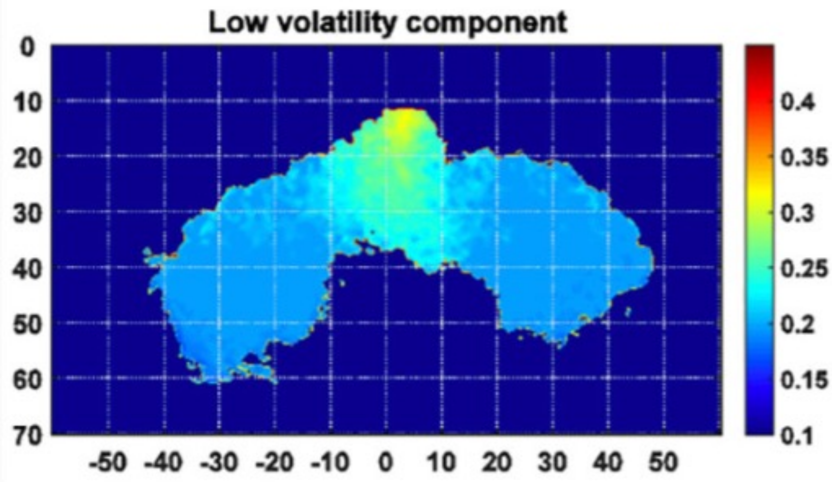
	G1
T_{fuel}(K)	363
$T_{ambient}$(K)	573
$p_{ambient}$(bar)	6

2 fuels:

- E00: n-pentane, iso-octane, n-undecane
- Pace 20:

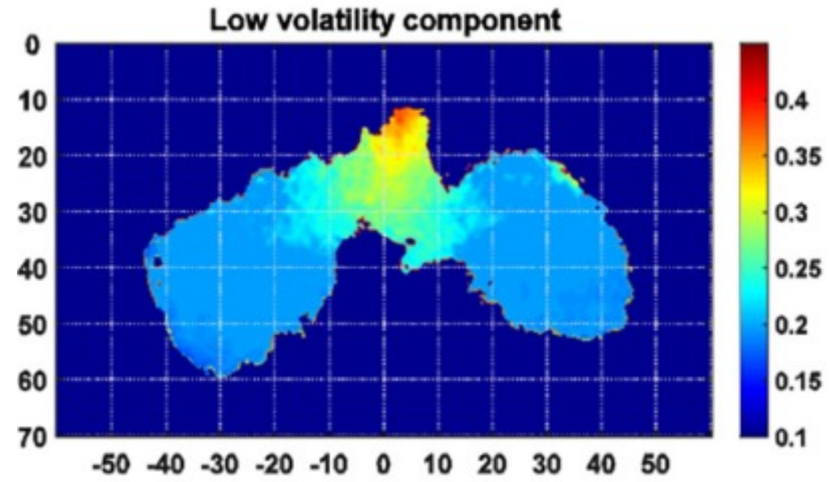
High-volatile fuels		Low-volatile fuels
iso-octane	1-hexene	toluene
n-pentane	n-heptane	1,2,4 trimethylbenzene
cyclopentane	ethanol	tetralin

Experimental Data [1] with E00



$Low\ volatility = \frac{m_{NC11H24}}{m_{fuel}}$

Experimental Data [1] with PACE20



[1] Cordier M et al., Quantitative measurements of preferential evaporation effects of multicomponent gasoline fuel sprays at ECN Spray G conditions. *IJER*. 2020

E00 FUEL – SPRAY COMPARISON

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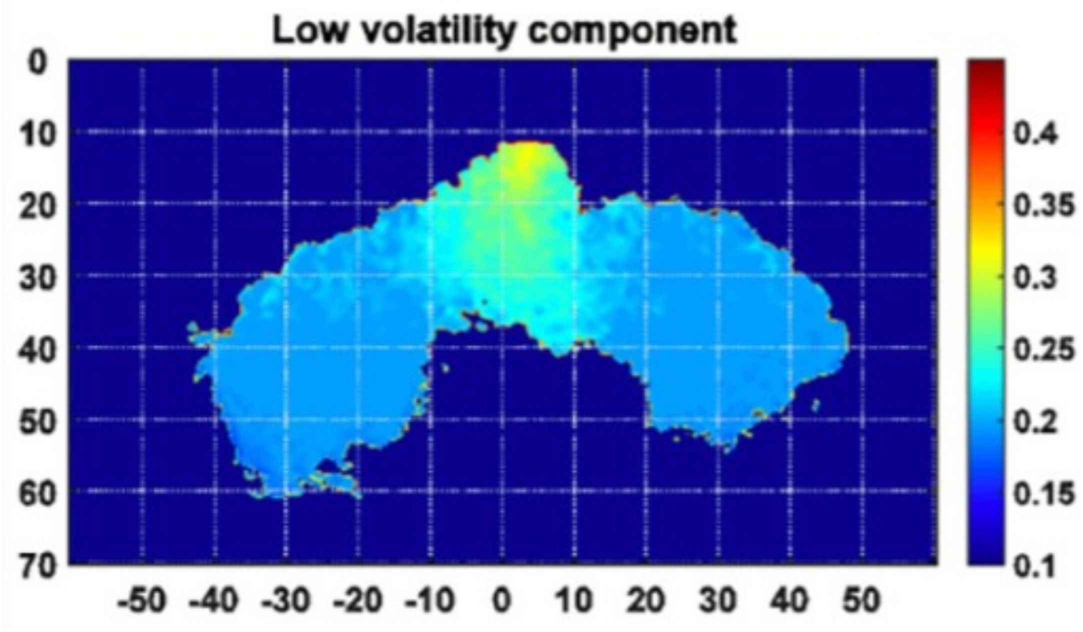
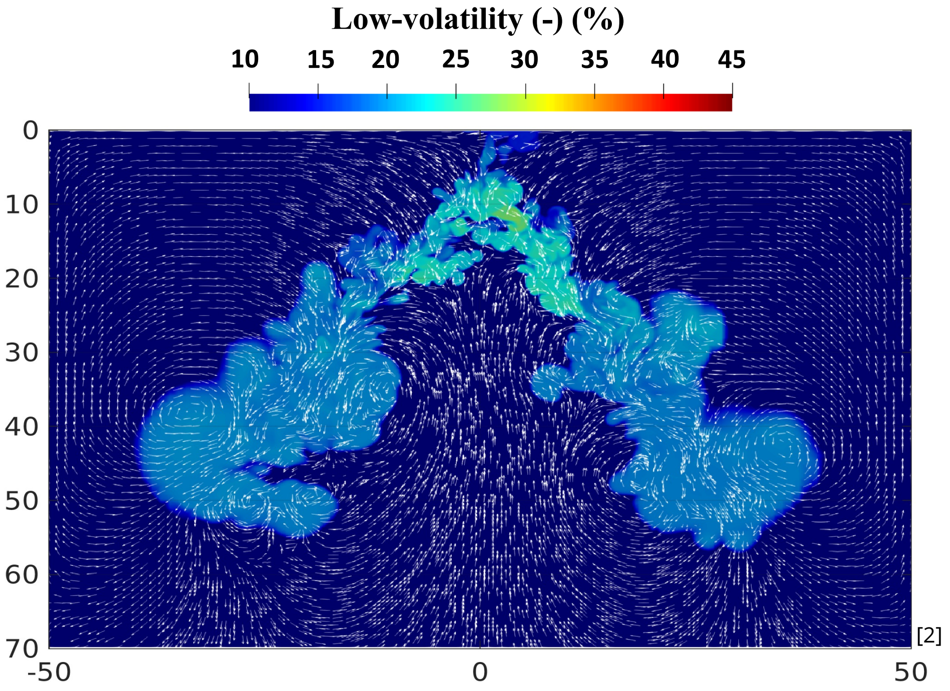
experimental Data [1]



simulation



- Low-volatility fuels are found towards the nozzle

[1] Cordier M et al., Quantitative measurements of preferential evaporation effects of multicomponent gasoline fuel sprays at ECN Spray G conditions. *IJER*. 2020
[2] Lien, Hao-Pin. Spray-wall-flow interaction within a gasoline direct-injection (GDI) engine using Large Eddy Simulation.. 2023

PACE 20 FUEL – SPRAY COMPARISON

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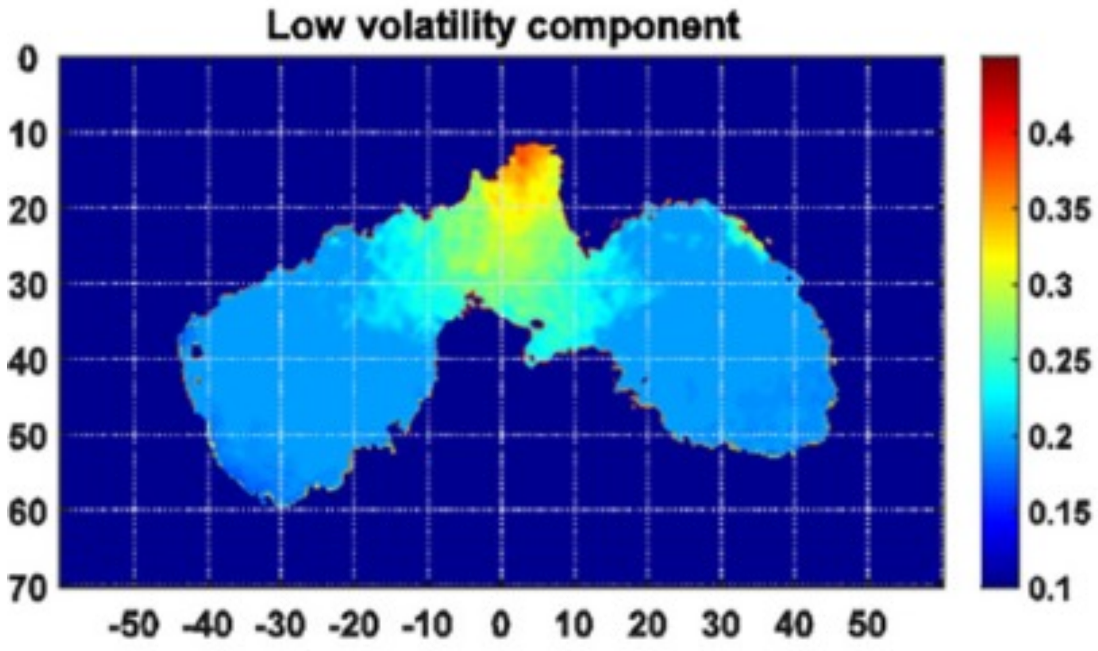
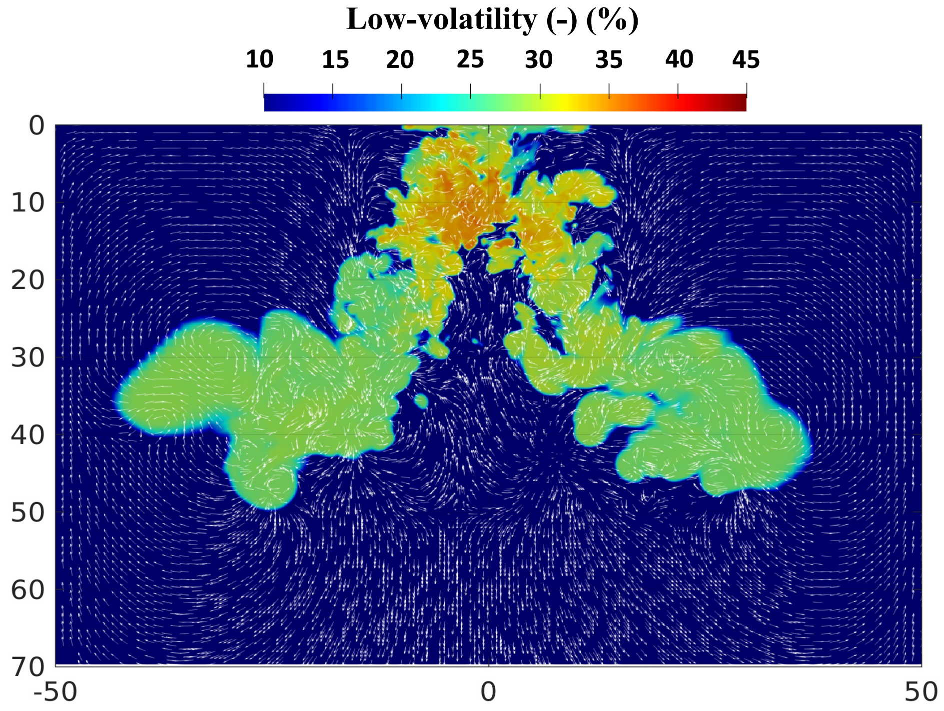
experimental Data [1]



simulation



- Addition of ethanol leads to further spatial separation of low- and high volatile components

[1] Cordier M et al., Quantitative measurements of preferential evaporation effects of multicomponent gasoline fuel sprays at ECN Spray G conditions. *IJER*. 2020
[2] Lien, Hao-Pin. Spray-wall-flow interaction within a gasoline direct-injection (GDI) engine using Large Eddy Simulation.. 2023

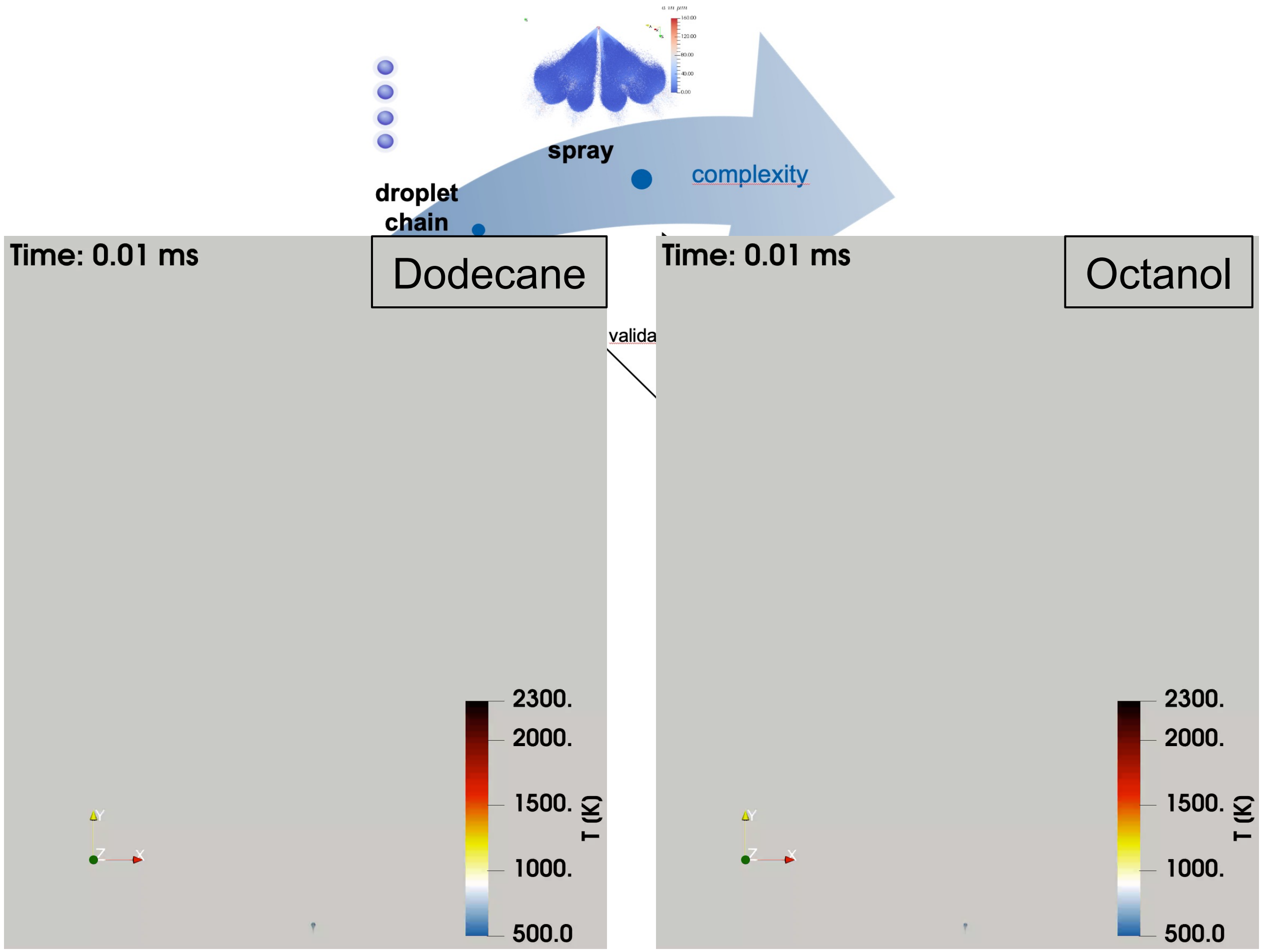
OUTLOOK & SUMMARY

summary:

- Modeling approach of evaporation of a VLE with real thermodynamics
- Increasing complexity accompanied by experiments

outlook:

- Investigation on influence of real VLE modeling in ethanol/iso-octane sprays
- Investigation into the combustion characteristics
  - Alcohol fuels have a higher latent heat of evaporation



[1] Haspel, Philip. Comparison of turbulent reactive spray characteristics of different renewable fuels using Large Eddy Simulation. 2023

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