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Motivation and Objective

Background

- Synthetic E-Fuels serve as blends in internal combustion engines (ICEs) thereby reducing greenhouse gases in the transport sector
 - Otto engine: Dimethylcarbonat (DMC), Methylformiat (MeFo)
 - Diesel engine: Oxymethylenether (OME)
- In ICEs, the in-cylinder pressure and temperatures vary widely, e.g. from 35 to 150 bar during Diesel fuel injection while the piston wall temperature ranges from 200°C to 500°C [1]
- Blending of gasoline and Diesel with E-fuels affects liquid properties while the gas density depends strongly on pressure and temperature

Scientific questions

▶ How do fuel properties and gas pressure affect drop wall interaction?

Objectives

- Study spreading of different fuels with respect to fluid dynamic similarity
- > Determine effect of gas-liquid density ratio on maximum spreading factor

Numerical Simulation

Diffuse-interface phase-field method [2]

- An energetic variational formulation based on continuum thermodynamics
- ▶ Interface is treated as a thin transition layer of finite and prescribed width
- ▶ Interface dynamics is modelled via the Cahn-Hilliard equation
- ▶ Fluid dynamics is modelled by the incompressible Navier-Stokes equations
- Implementation in OpenFOAM (FOAM-extend, code phaseFieldFoam)

Numerical setup and parameters

- ► Wedge type axisymmetric geometry (wedge angle 4°)
- ▶ Fixed grid, Cahn number 0.02, diffuse interface resolved by 13 mesh cells
- Impact parameters chosen below splashing limit [3]
 - Fixed Weber number $We = \rho_L DU^2 / \sigma = 150$
 - Fixed Reynolds number $Re = \rho_L DU/\mu_L = 900$
 - ► The variation in fuel properties results in variation of drop diameter $(D=\mu_L^2Re^2/\sigma_{P_L}We)$, drop impact velocity $(U=\sigma We/\mu_L Re)$, gas-liquid density ratio (ρ_G/ρ_L) and gas-liquid viscosity ratio (μ_G/μ_L)

z

DU

Axis

Drop

Atmosphere

2 5D

Side

2.5D

Physical properties

- Liquid fuels (at room temperature)
 - Gasoline (RON95) [4]
 - Pure DMC [4]
 - Pure MeFo [4]
 - Pure OME (OMDME₃) [5]
- Gas properties
 - ▶ $\rho_{\rm G} = \{1.2, 12, 24, 36\} \text{ kg/m}^3$
 - $v_{\rm G} = \mu_{\rm G} / \rho_{\rm G} = 15.2 \text{ mm}^2/\text{s}$ (fixed)
 - Wall contact angle 50° (fixed) Fig. 1: Sketch of computational domain.

Liquid fuel	ρ _ [kg/m³]	μ_{L} [mPa s]	σ [mN/m]	<i>D</i> [µm]	<i>U</i> [m/s]
RON95	746	0.395	20.0	57.0	8.4
DMC	1073	0.722	28.5	92.1	6.6
MeFo	980	0.354	25.0	27.6	11.8
OME (OMDME ₃)	1031	1.110	28.8	225.0	4.3

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Results

Effect of liquid fuel properties at fixed pressure (gas density)

- Normalization of instantaneous spreading radius by initial drop radius
- ► Normalization of time by kinematic time scale D/U
- Effect of fuel properties is small for 1 bar but increases with pressure



Fig. 2: Effect of fuel properties on instantaneous spreading factor for gas densities corresponding to 1 bar (left) and to 20 bar (right).

Effect of gas density due to variation of ambient pressure

- Increase of gas density dampens receding after maximum spreading
- Maximum spreading slightly decreases with increase of gas density
- For all fuels, the maximum spreading factors for 1 bar agree well with an empirical correlation from [6] but deviate for larger gas densities



Fig. 3: Effect of gas density on instantaneous spreading of DMC (left) and on maximum spreading (right) compared with an empirical correlation [6].

Conclusions

- Numerical study on the effects of fuel properties and gas density for fixed values of Weber number, Reynolds number and wall contact angle
- At gas density equivalent to 1 bar, maximum spreading is only slightly affected by fuel properties and well described by a literature correlation
- An increase of gas density (i.e. gas inertia) reduces maximum spreading slightly and dampens spreading dynamics during receding
- Standard spreading correlations can be used for blends with E-fuels but may be extended to account for the gas-liquid density ratio

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Turbulent, chemically reactive

multi-phase flows near walls

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