Numerical Simulation of Bubble Dynamics and Local Segregation in Binary Dodecane/Heptane mixtures

Kavitationsworkshop Drübeck

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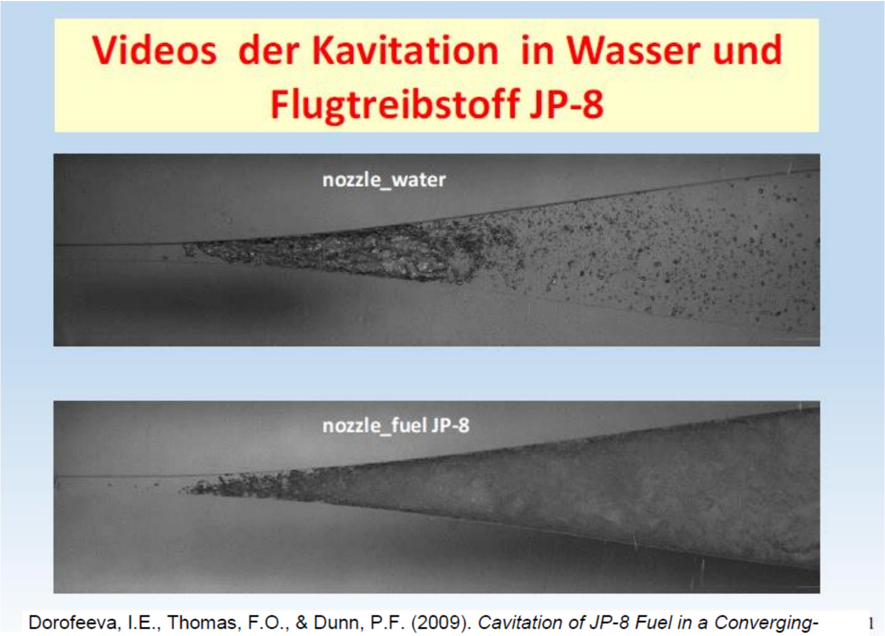
Motivation

- Appearance of cavitation in mixtures cannot be captured by 3D simulation

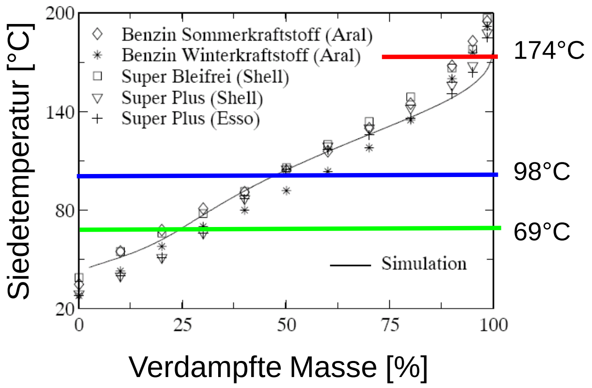
- Task: Development of multi-component cavitation models.

- 1. step: **Multi-component Single Bubble Model**
  - Coupled mass and heat transfer
  - Segregated evaporation of alcane mixtures
  - Keep it simple:
    Binary alcane mixtures



Dorofeeva, I.E., Thomas, F.O., & Dunn, P.F. (2009). *Cavitation of JP-8 Fuel in a Converging-Diverging Nozzle: Experiments and Modelling*. Proc. 7th Int. Symp. Cavitation.
Dunn, P.F., Thomas, F.O., Davis, M.P., & Dorofeeva, I.E. (2010). *Experimental characterization of aviation-fuel cavitation*. Phys. Fluids, 22, 117102.

Destillation curve



n-Hexan

n-Heptan

n-Dekan

Assumptions and governing equations

- Sperical single bubble
- Binary mixture of heptane and dodecane / dissolved + free air
- Conservation of mass (species transport) and energy, within + outside bubble

$$\frac{\partial\left(\rho_{\mathrm{m}}^{\gamma} y_{\alpha}^{\gamma}\right)}{\partial t}+\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \rho_{\mathrm{m}}^{\gamma} y_{\alpha}^{\gamma} u^{\gamma}\right)=\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \rho_{\mathrm{m}}^{\gamma} D_{\alpha}^{\gamma} \frac{\partial y_{\alpha}^{\gamma}}{\partial r}\right)$$

$$\frac{\partial\left(\rho_{\mathrm{m}}^{\mathrm{G}} e_{\mathrm{m}}^{\mathrm{G}}\right)}{\partial t}+\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \rho_{\mathrm{m}}^{\mathrm{G}} h_{\mathrm{m}}^{\mathrm{G}} u^{\mathrm{G}}\right)=-\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} q^{\mathrm{G}}\right)$$

- Within bubble: (Spatially resolved) Momentum balance is substituted by energy balance [1,2]
  - For $p_G = konst.|_r$ (homobaricity) we obtain an analytical expression for velocity field and pressure:

$$u^{\mathrm{G}}=-\frac{r}{3 p^{\mathrm{G}}} \frac{\mathrm{d} p^{\mathrm{G}}}{\mathrm{d} t}+\frac{1}{r^{2} p^{\mathrm{G}}} \int_{0}^{r}\left(G(r)+\frac{\Re_{\mathrm{m}}}{c_{p, \mathrm{m}}^{\mathrm{G}}} \frac{\mathrm{d} p^{\mathrm{G}}}{\mathrm{d} t}\right) r^{2} \mathrm{d} r$$

$$\frac{\mathrm{d} p^{\mathrm{G}}}{\mathrm{d} t}=\frac{-R^{2} p^{\mathrm{G}} u_{\mathrm{w}}^{\mathrm{G}}+\int_{0}^{R} G(r) r^{2} \mathrm{d} r}{\frac{R^{3}}{3}-\int_{0}^{R} \frac{\Re_{\mathrm{m}}}{c_{p, \mathrm{m}}^{\mathrm{G}}} r^{2} \mathrm{d} r}$$

$$\begin{aligned} G(r)=\frac{\Re_{\mathrm{m}}}{c_{p, \mathrm{m}}^{\mathrm{G}}}\Bigg\{ & \frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \rho_{\mathrm{m}}^{\mathrm{G}} T^{\mathrm{G}} \sum_{\alpha=1}^{N_{\mathrm{S}}} \Re_{\alpha} D_{\alpha}^{\mathrm{G}} \frac{\partial y_{\alpha}^{\mathrm{G}}}{\partial r}\right)+\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \lambda_{\mathrm{m}}^{\mathrm{G}} \frac{\partial T^{\mathrm{G}}}{\partial r}\right) \\ & +\frac{T^{\mathrm{G}} c_{v, \mathrm{m}}^{\mathrm{G}}}{\Re_{\mathrm{m}}} \frac{1}{r^{2}} \sum_{\alpha=1}^{N_{\mathrm{S}}} \Re_{\alpha} \frac{\partial}{\partial r}\left(r^{2} \rho_{\mathrm{m}}^{\mathrm{G}} D_{\alpha}^{\mathrm{G}} \frac{\partial y_{\alpha}^{\mathrm{G}}}{\partial r}\right)+\rho_{\mathrm{m}}^{\mathrm{G}} \frac{\partial T^{\mathrm{G}}}{\partial r} \sum_{\alpha=1}^{N_{\mathrm{S}}} c_{v, \alpha}^{\mathrm{G}} D_{\alpha}^{\mathrm{G}} \frac{\partial y_{\alpha}^{\mathrm{G}}}{\partial r}\Bigg\}\end{aligned}$$

- Outside bubble: Potential flow

[1] Nigmatulin, R.I. et al.(1981). Int. J. Heat Mass Transfer, 24(6)
[2] Kawashima, H. et al. (2008). J. Fluid Science Technology, 3(8), 943-955

Assumptions and governing equations

- Bubble wall location by extended Rayleigh-Plesset equation with mass transfer [1)]

$$R\ddot{R}\left(1-2\frac{\dot{R}}{a^{L}_{m,w}}+\frac{\dot{m}''}{\rho^{L}_{m,w}a^{L}_{m,w}}\right)+\frac{3}{2}\dot{R}^{2}\left(1+\frac{4}{3}\frac{\dot{m}''}{\rho^{L}_{m,w}a^{L}_{m,w}}-\frac{4}{3}\frac{\dot{R}}{a^{L}_{m,w}}\right)$$
$$-\frac{\dot{m}''R}{\rho^{L}_{m,w}}\left(1-2\frac{\dot{R}}{a^{L}_{m,w}}+\frac{\dot{m}''}{\rho^{L}_{m,w}a^{L}_{m,w}}\right)-\frac{\dot{m}''}{\rho^{L}_{m,w}}\left(\dot{R}+\frac{\dot{m}''}{2\rho^{L}_{m,w}}\right)$$
$$+\left(\frac{p^{L}_{\infty}-p^{L}_{w}}{\rho^{L}_{m,w}}\right)+\left(\frac{R}{\rho^{L}_{m,w}a^{L}_{m,w}}\right)\frac{d}{dt}\left(p^{L}_{\infty}-p^{L}_{w}\right)=0$$

- Henry law

$$y^{L}_{Air,w}=\frac{M_{Air}}{M^{L}_{m,w}H_{m}}\,y^{G}_{Air,w}\,\frac{\mathfrak{R}_{Air}}{\mathfrak{R}_{m,w}}\,p^{G}$$

- Thermal and chemical equilibrium at bubble wall

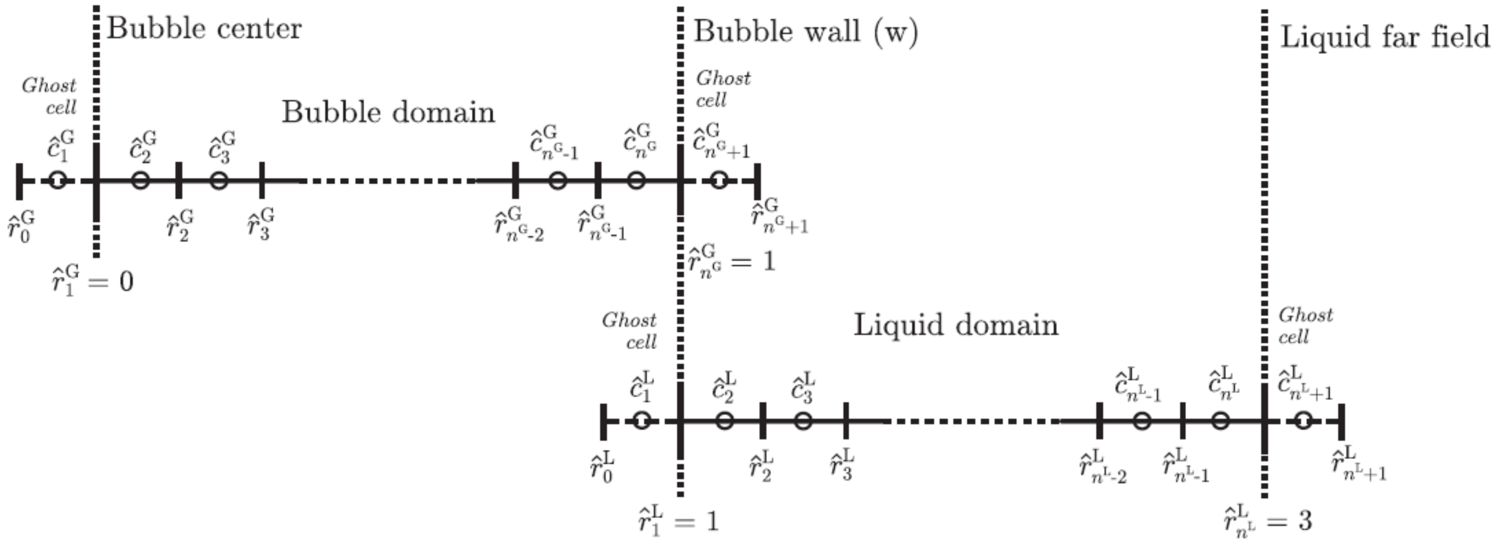
$$T^{G}_{w}=T^{L}_{w}$$

$$y^{L}_{\alpha,w}\frac{M^{L}_{m,w}}{M_{\alpha}}\,p^{Sat}_{\alpha}\Big|_{T^{L}_{w}}=y^{G}_{\alpha,w}\frac{M^{G}_{m,w}}{M_{\alpha}}p^{G}$$

1) Fujikawa, S. & Akamatsu, T. (1980). J. Fluid Mech., 97, 481-512

Numerical solution

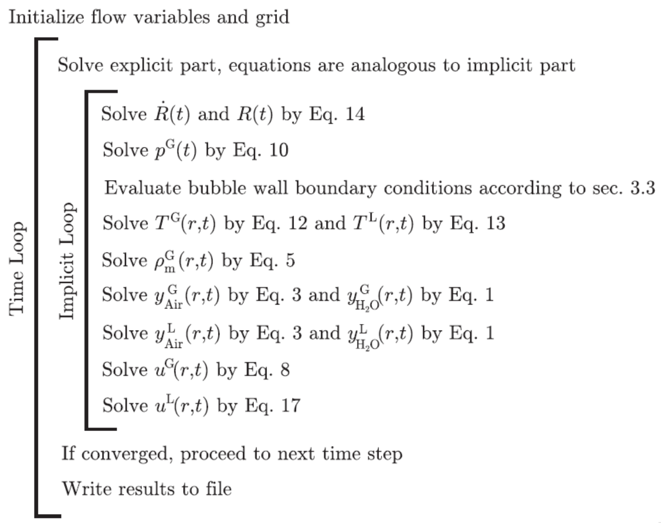
- Combined Finite Volume / Finite Difference scheme
  - Staggered and moving grid



- Thermophysical properties adopted from droplet evaporation models

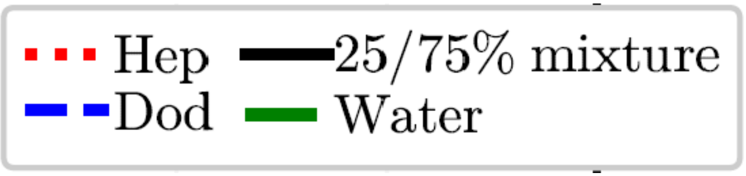
- Crank-Nicolson scheme for time discretisation

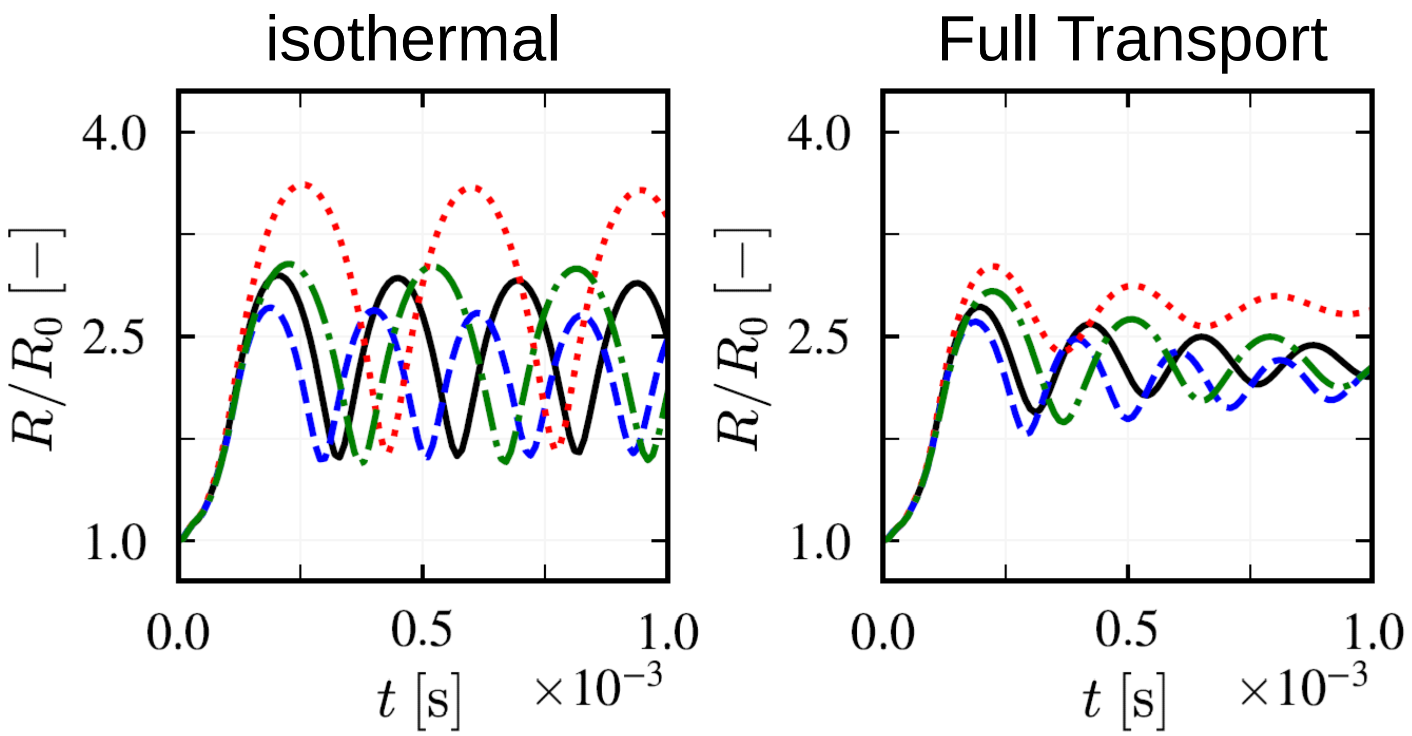
- Coded in F90 from scratch



1. Test case: sudden pressure drop

- R_0 = 100 μm, T_0 = 293 K
- Drop from 10^5 Pa to 10^4 Pa, no cavitation
- **25 % heptane, 75 % dodecane <u>in liquid</u>**
- Effect of transport processes:

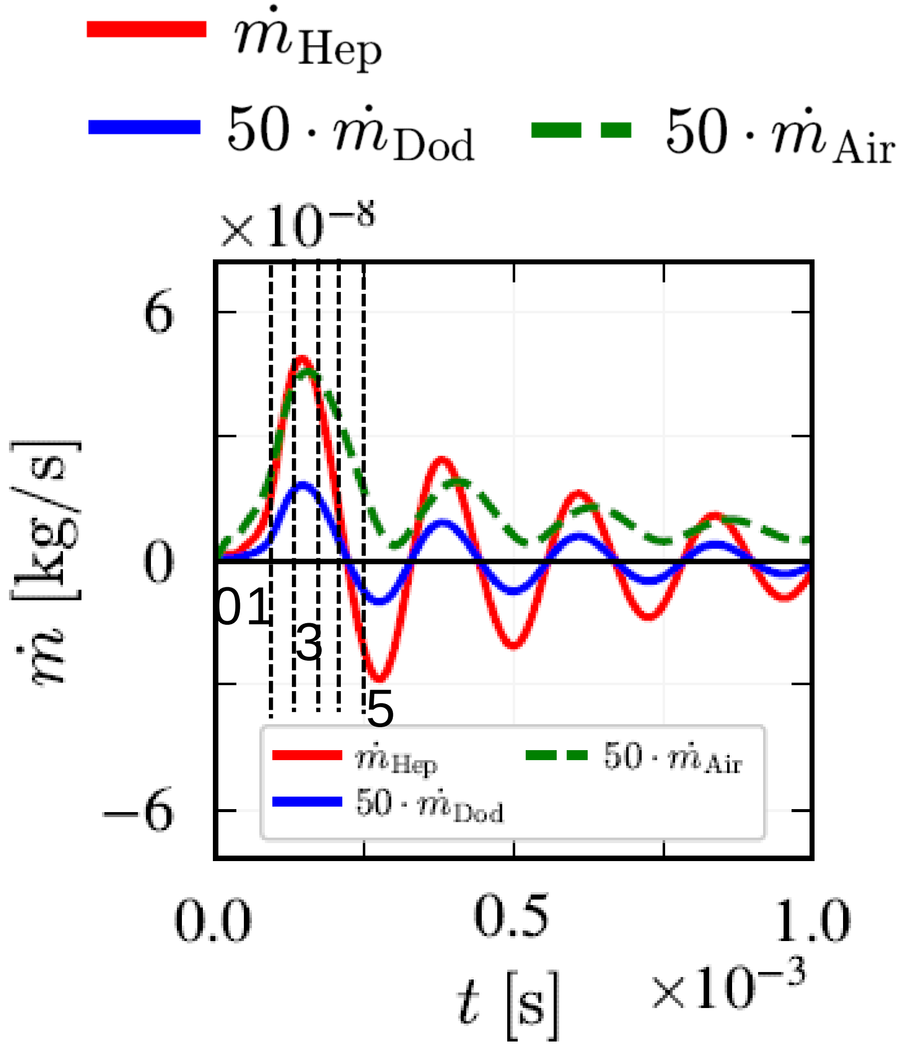




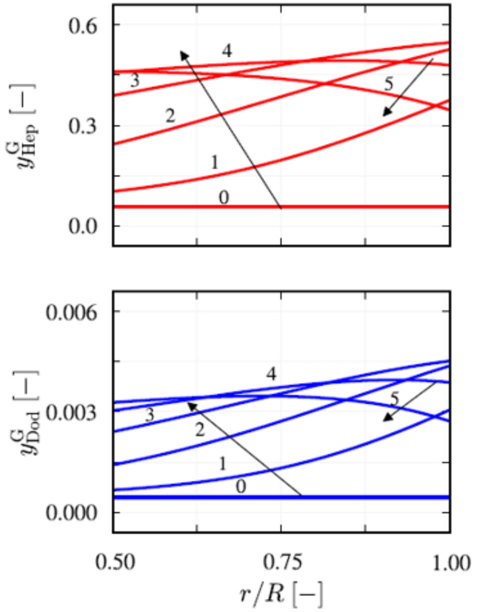
Thermal damping!

1. Test case: sudden pressure drop

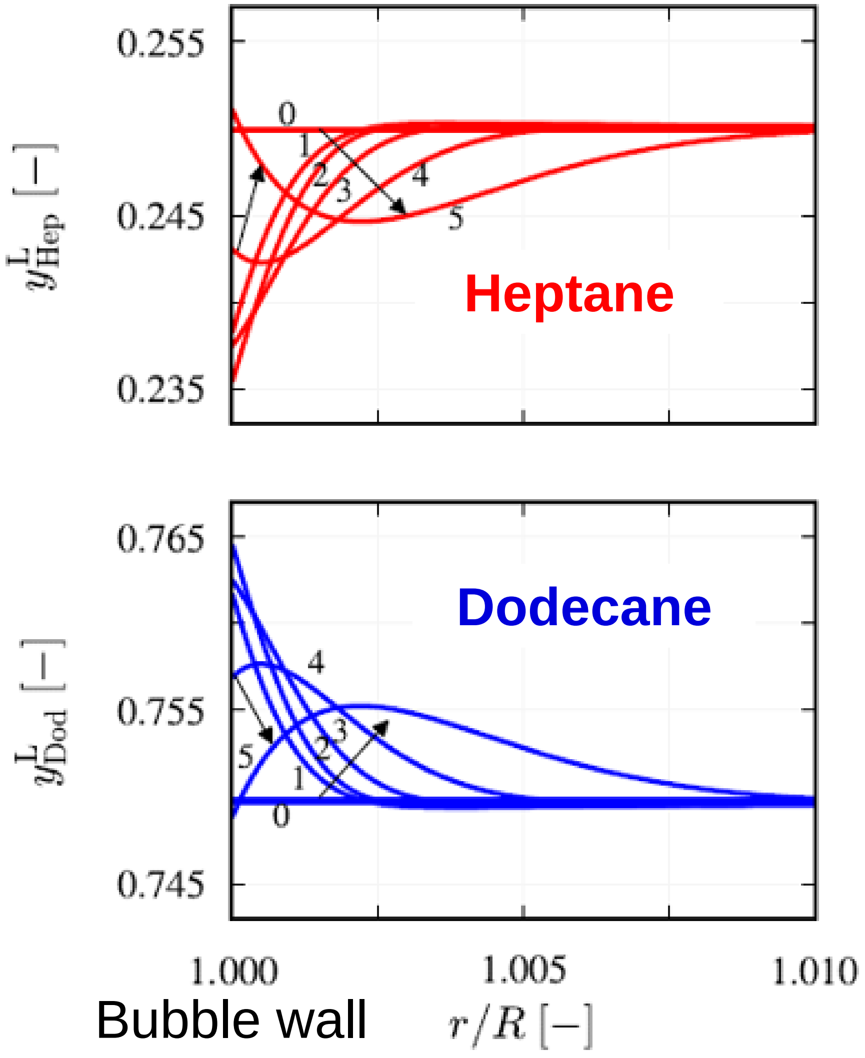
- Segregated mass transfer



Mass fraction in bubble



Mass fraction in liquid

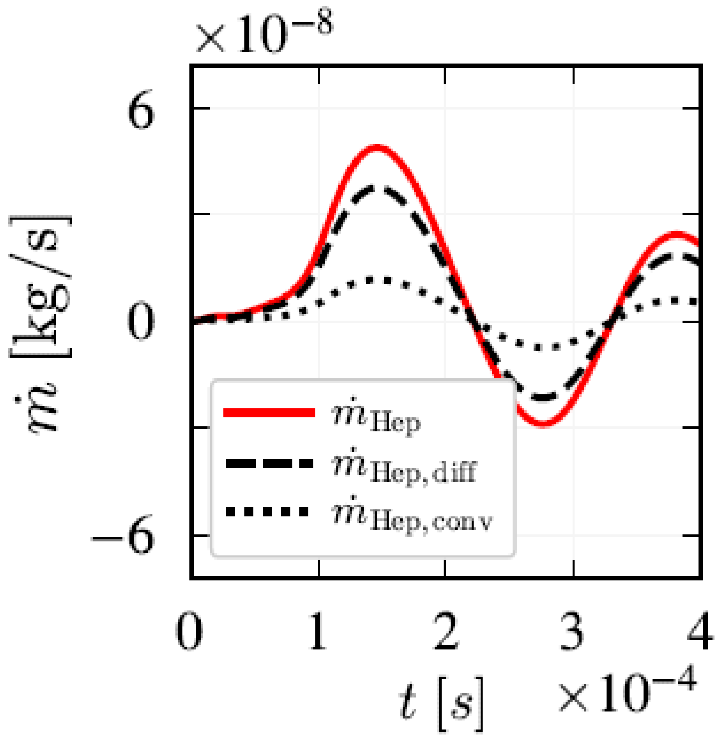


1. Test case: sudden pressure drop

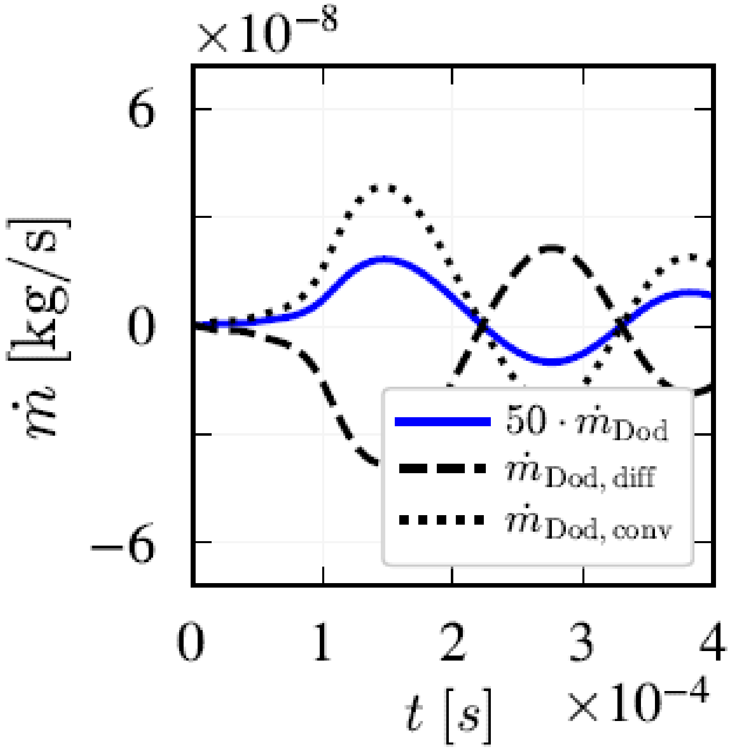
- Specific Mass fluxes

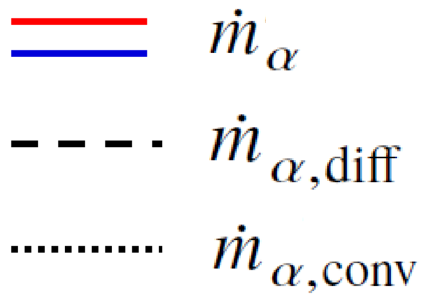
$$\dot{m}''_{\alpha} = \dot{m}''_{\alpha,\mathrm{conv}} + \dot{m}''_{\alpha,\mathrm{diff}} = \underbrace{-\rho^{\mathrm{L}}_{\mathrm{m,w}} y^{\mathrm{L}}_{\alpha,\mathrm{w}} (u^{\mathrm{L}}_{\mathrm{w}} - \dot{R})}_{\dot{m}''_{\alpha,\mathrm{conv}}} + \underbrace{\rho^{\mathrm{L}}_{\mathrm{m,w}} D^{\mathrm{L}}_{\alpha,\mathrm{w}} \left.\frac{\partial y^{\mathrm{L}}_{\alpha}}{\partial r}\right|_{\mathrm{w}}}_{\dot{m}''_{\alpha,\mathrm{diff}}}$$

Heptane



Dodecane



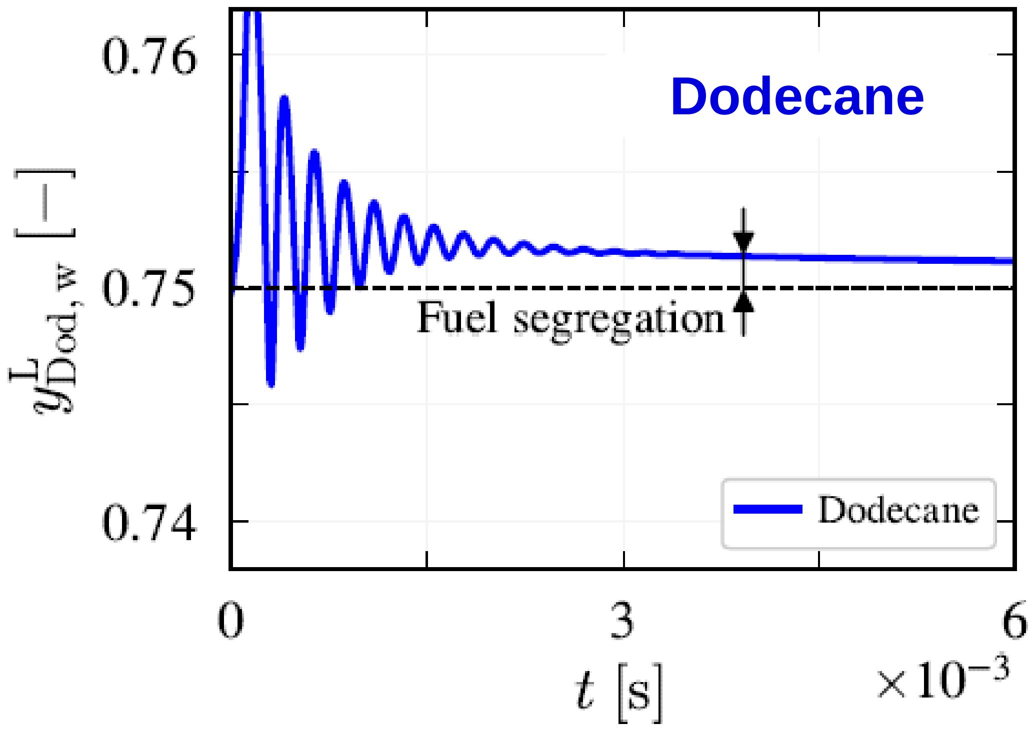


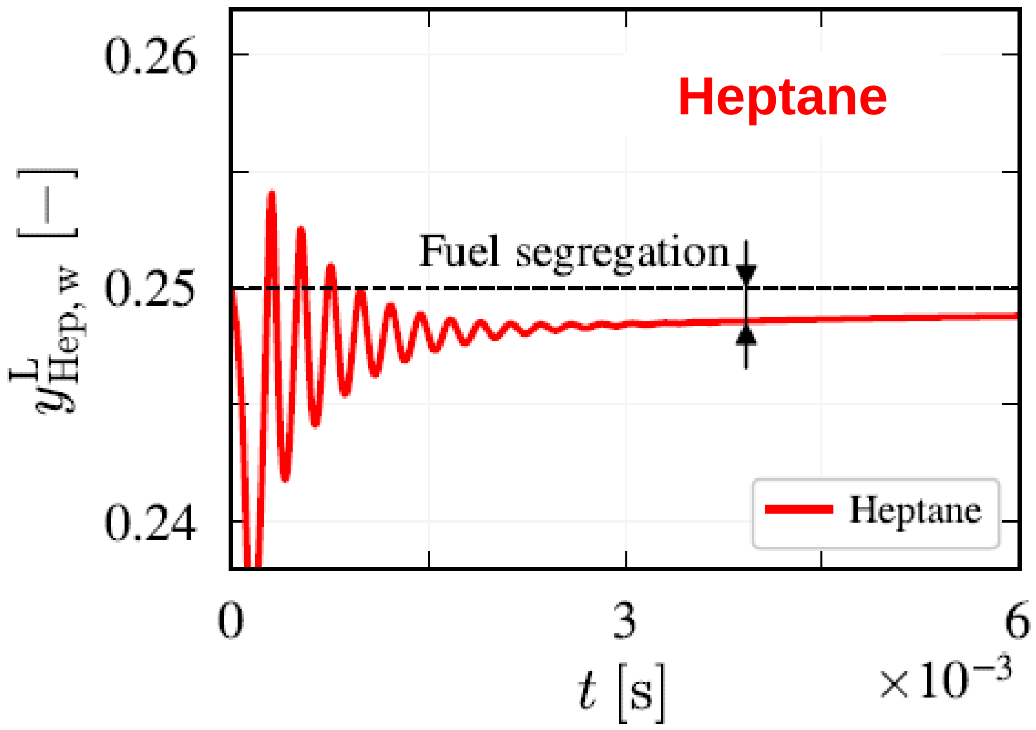
- **Low-Volatile** Species: convective and diffusive mass flux always **opposite**.
- **High-volatile** Species: convective and diffusive mass flux always **in same direction**.

1. Test case: sudden pressure drop

➢ Local segregation in the liquid

Species Wall Concentration on **liquid side** of bubble wall:





➢ By comparing with a **non-segregatable pseudo-fluid**: (results not shown)

➢ Local segregation has no effect on bubble dynamics!
➢ Is this observation test-case specific?

2. Test case: bubble growth in superheated liquid

- Bubble growth in superheated water

- $t < t_{C1}$ small: **inertia controlled** growth (**Rayleigh**)
- $t > t_{C1}$ small: **thermally controlled** growth (**Plesset-Zwick**)

$$t_{c1} = \Delta p_{\mathrm{Tension}} / (\rho_{\mathrm{m}}^{\mathrm{L}} \Sigma^2)$$

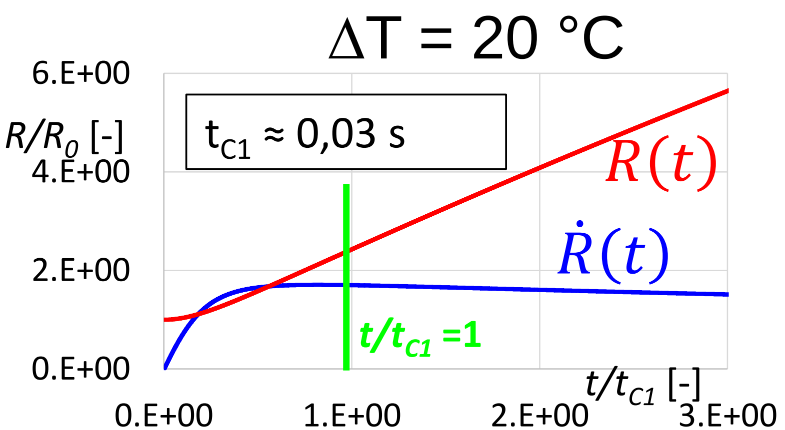
- Thermodynamic parameter

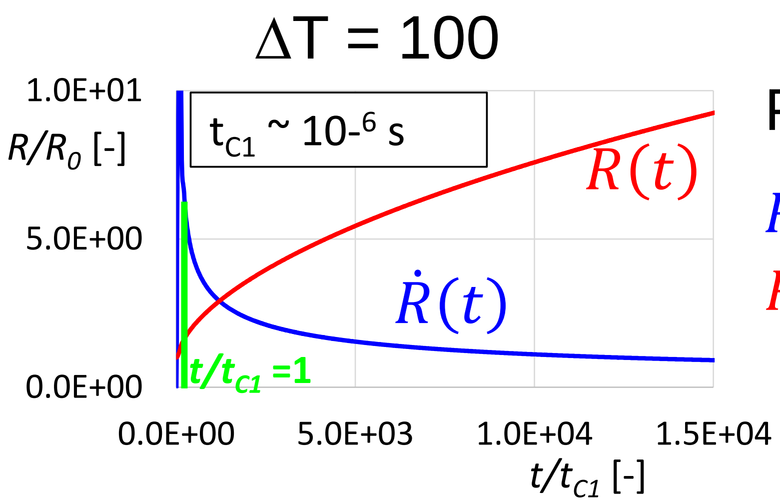
$$\Sigma = \frac{\left[L_{\mathrm{m}} \rho_{\mathrm{m,w}}^{\mathrm{G}}\right]^2}{T_0^{\mathrm{L}} \sqrt{(\rho_{\mathrm{m}}^{\mathrm{L}})^3 c_{\mathrm{m}}^{\mathrm{L}} \lambda_{\mathrm{m}}^{\mathrm{L}}}}$$

Rayleigh

$\dot{R} \sim const.$

$R \sim t$





Plesset-Zwick

$\dot{R} \sim t^{-0,5}$

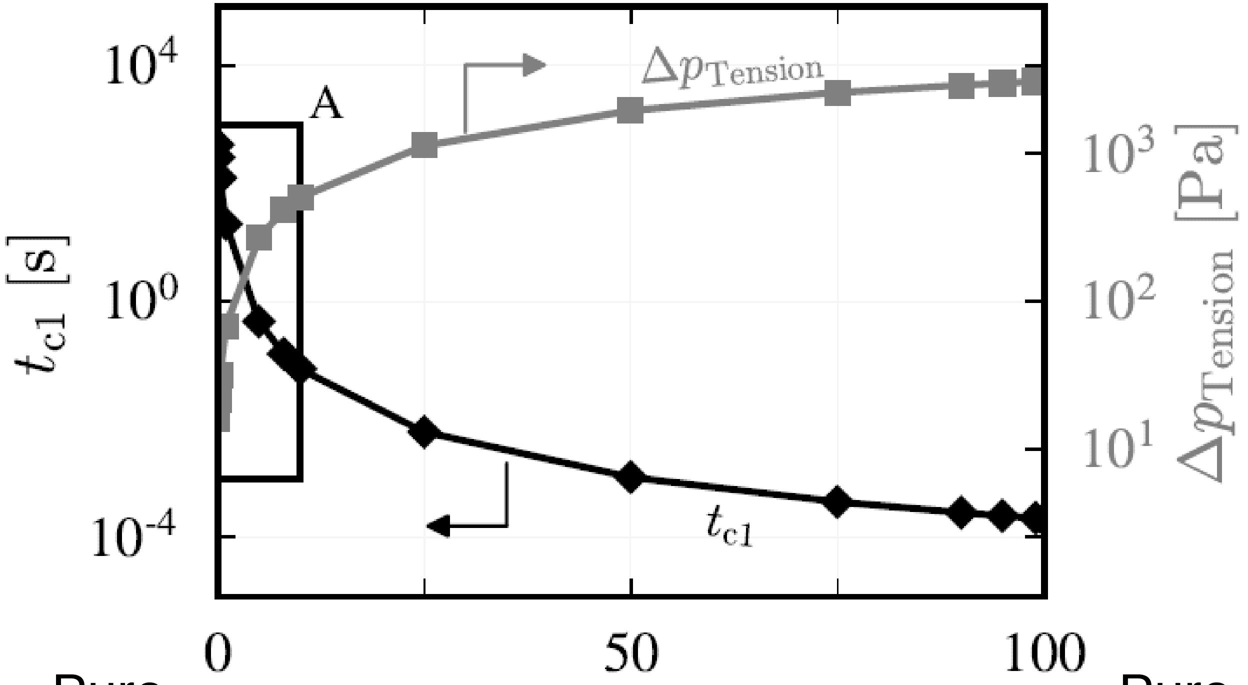
$R \sim t^{0,5}$

2. Test case: bubble growth in superheated liquid

- Heptane / Dodecane mixture, R_0 = 100 μm
- Constant superheat level $\Delta T_{\mathrm{SH}} = 10\,\mathrm{K}$ at T_0 = 30°C
  - $\Delta p_{\mathrm{Tension}}$ and t_{c1} vary with mixture composition!

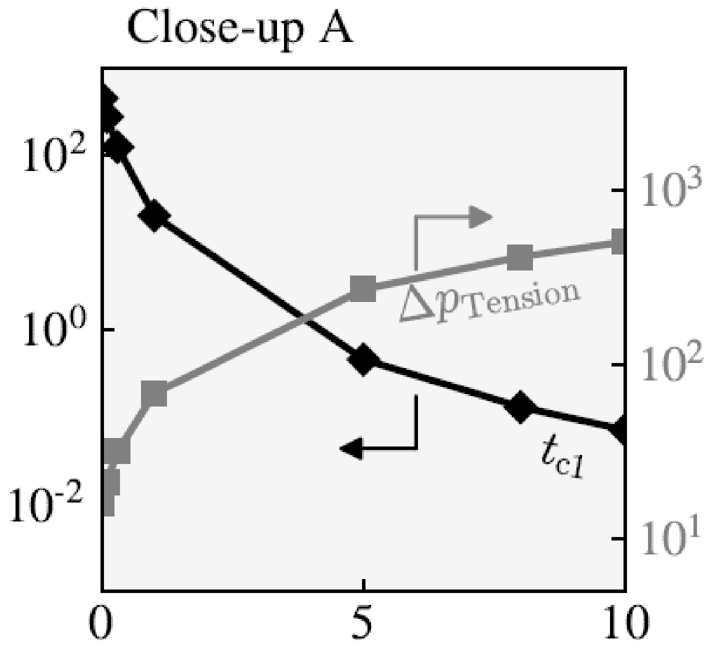
$$t_{\mathrm{c1}} = \Delta p_{\mathrm{Tension}} / (\rho_{\mathrm{m}}^{\mathrm{L}}\, \Sigma^2)$$

$$\Sigma = \frac{\left[L_{\mathrm{m}} \rho_{\mathrm{m,w}}^{\mathrm{G}}\right]^2}{T_0^{\mathrm{L}} \sqrt{(\rho_{\mathrm{m}}^{\mathrm{L}})^3 c_{\mathrm{m}}^{\mathrm{L}} \lambda_{\mathrm{m}}^{\mathrm{L}}}}$$



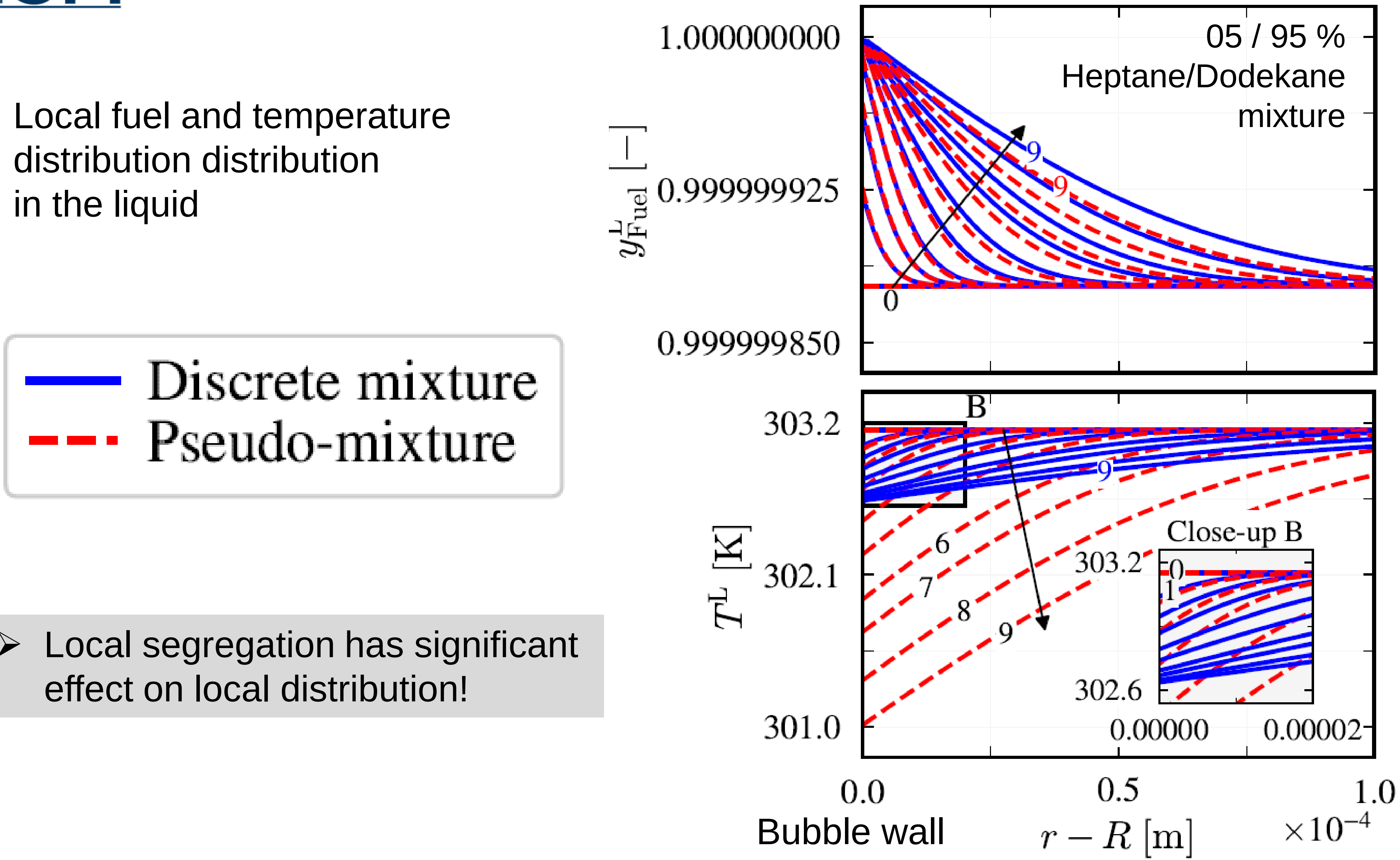
Pure Heptane

Pure Dodecane



2. Test case: bubble growth in superheated liquid

- Local fuel and temperature distribution distribution in the liquid

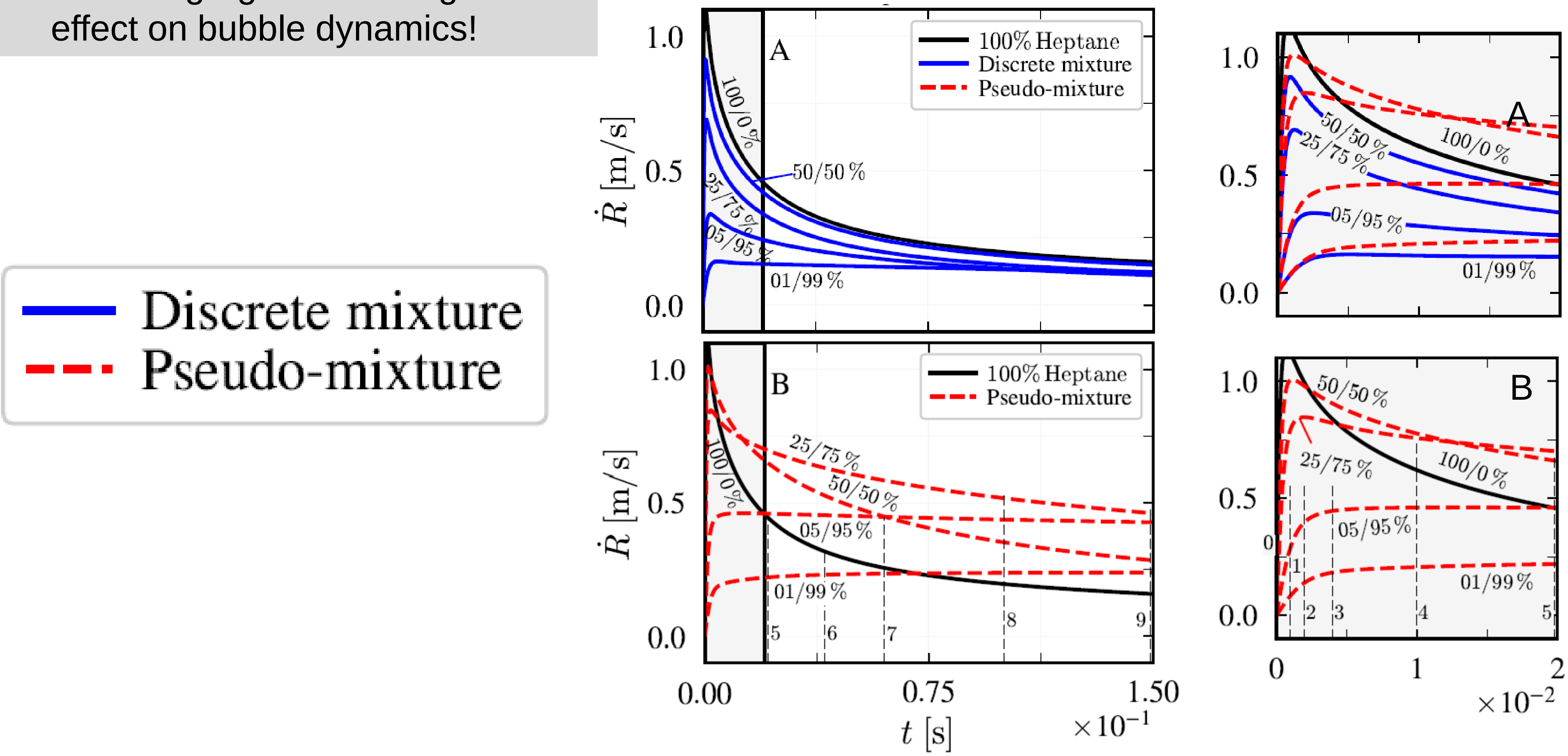


- **Local segregation has significant effect on local distribution!**

2. Test case: bubble growth in superheated liquid

- ➢ Local segregation has significant effect on bubble dynamics!

Different heptan/dodecane mixture ratios

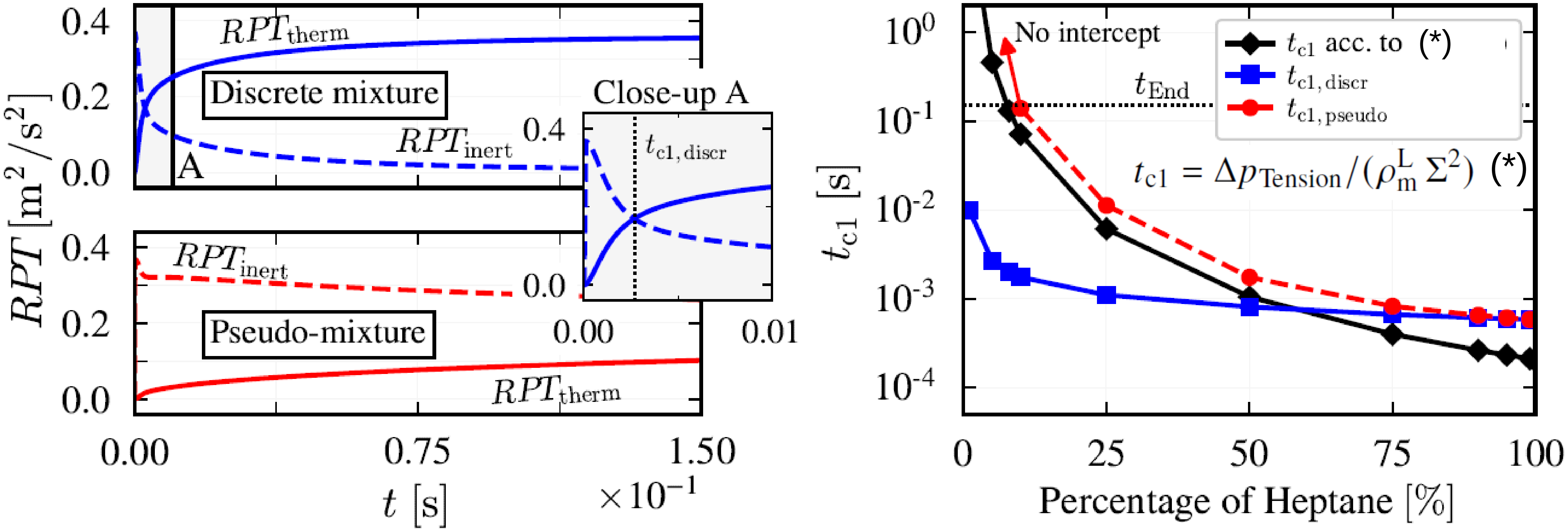


2. Test case: bubble growth in superheated liquid

➢ Inertia and thermal term
in Rayleigh-Plesset equation

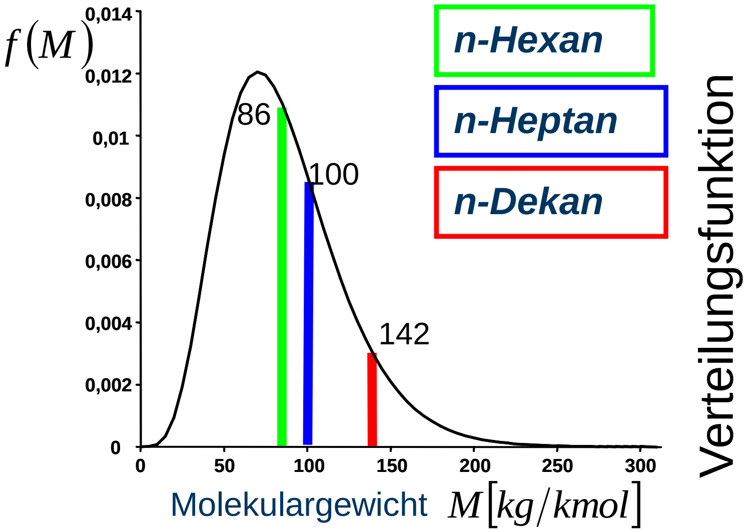
$$RPT_{\mathrm{inert}} = R\ddot{R} + \frac{3}{2}\dot{R}^2 \qquad RPT_{\mathrm{therm}} = \frac{p_{\mathrm{m}}^{\mathrm{Sat}}\big|_{T_0^{\mathrm{L}}} - p_{\mathrm{m}}^{\mathrm{Sat}}\big|_{T_{\mathrm{W}}^{\mathrm{L}}}}{\rho_{\mathrm{m}}^{\mathrm{L}}}$$

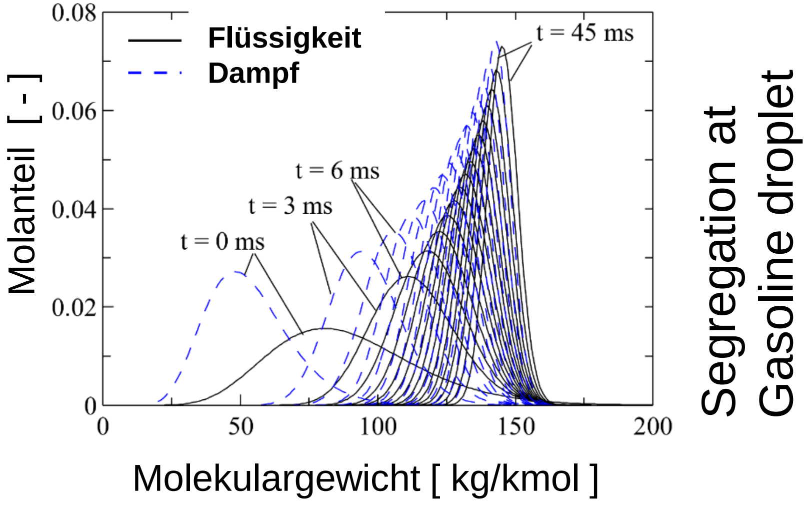
Example: 05/95 % heptane/dodekane mixture



➢ For the real (discrete) mixture the thermally-controlled growth starts much earlier than for the pseudo mixture!

- Next steps:
  - Real fuels with continuous thermodynamics





  - Coupling to 3D CFD
    - Euler-Lagrange
  - Experiments!

Thank you for your attention!

Thanks to our sponsor for funding.