On multicomponent two-phase flows with mass transfer

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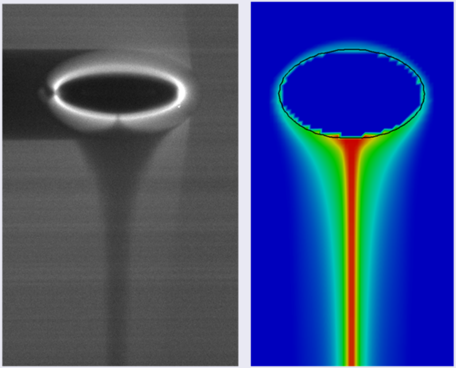
joint work with Jan Prüss

Motivation

Mass transfer from rising bubbles

Oxygen concentration around a rising air bubble



gas bubble:
O_2, N_2, CO_2,
water vapor

ambient liquid:
water,
O_2, N_2, CO_2

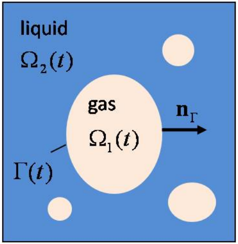
Sharp interface model

Continuum mechanical model with sharp interface

- captures the relevant macroscopic phenomena in many cases

Two-phase system

- continuous physical quantities inside the bulk phases
- jump discontinuities at the phase boundaries



Multicomponent system

- mixture of several chemical components
- partial miscibility

Multicomponent single-phase fluid mixture

chemical components $A_1, \dots, A_n$, possibly with chemical reactions

individual mass balances:

$$\partial_t \rho_i + \operatorname{div}(\rho_i \mathbf{u}_i) = M_i\, r_i^{\text{tot}} \quad \text{in } \Omega$$

$\rho_i = \rho_i(t,x)$	individual mass densities
$\mathbf{u}_i = \mathbf{u}_i(t,x)$	individual velocity fields
M_i	molar mass of species i
r_i^{tot}	molar rate of change due to chemical reactions
$\Omega \subset \mathbb{R}^n$	open domain with smooth boundary $\partial\Omega$

common variant: use molar concentrations $c_i := \rho_i / M_i$.

$$\partial_t c_i + \operatorname{div}(c_i \mathbf{u}_i) = r_i^{\text{tot}} \quad \text{in } \Omega$$

Multicomponent single-phase fluid mixture

assumption: isothermal conditions

individual momentum balances*:

$$\partial_t(\rho_i \mathbf{u}_i) + \nabla \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) = -\, c_i \nabla \mu_i + \nabla \cdot \mathbf{S}_i + \rho_i \mathbf{F}_i - c^{\mathrm{tot}} R\,T \sum_{j \neq i} f_{ij}\, x_i\, x_j (\mathbf{u}_i - \mathbf{u}_j) \quad \text{in } \Omega$$

μ_i	chemical potential of species i
$\mathbf{S}_i$	viscous stress of species i
$\mathbf{F}_i$	body forces acting on species i
c^{tot}	sum of all molar concentrations
$R\,T$	universal gas constant times absolute temperature
f_{ij}	friction factor for collisions between species i, j; $f_{ij} = f_{ji} > 0$
x_i	molar fraction of species i; $x_i = c_i / c^{\mathrm{tot}}$

* P. Kerkhof, TU/e

Multicomponent single-phase fluid mixture

mixture balances

$$\rho := \sum_i \rho_i, \qquad \rho \mathbf{u} := \sum_i \rho_i \mathbf{u}_i \quad (\Rightarrow \text{barycentric velocity } \mathbf{u})$$

continuity equation: (conservation of total mass, i.e. $\sum_i M_i r_i^{\text{tot}} = 0$)

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \quad \text{in } \Omega$$

individual mass balances:

$$\partial_t \rho_i + \operatorname{div}(\rho_i \mathbf{u} + \mathbf{j}_i) = M_i\, r_i^{\text{tot}} \quad \text{in } \Omega$$

with molecular fluxes $\mathbf{j}_i = \rho_i(\mathbf{u}_i - \mathbf{u})$ which need to be modeled.

Multicomponent single-phase fluid mixture

balance of total momentum:

for simplicity: no external forces

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\sum_i c_i \nabla \mu_i + \nabla \cdot \sum_i \left(\mathbf{S}_i + \frac{1}{\rho_i} \mathbf{j}_i \otimes \mathbf{j}_i \right)$$

Note: $\nabla_T \mu_i = \nabla_{T,p} \mu_i + v_i \nabla p$

with $v_i = \frac{\partial \mu_i}{\partial p}$ the partial molar volume, p the total pressure

Gibbs-Duhem: $\sum_i c_i \nabla_T \mu_i = \nabla p$

$$\boxed{\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S}}$$

with the mixture stress tensor $\mathbf{S} = \sum_i \left(\mathbf{S}_i + \frac{1}{\rho_i} \mathbf{j}_i \otimes \mathbf{j}_i \right)$

Multicomponent single-phase fluid mixture

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Multicomponent single-phase fluid mixture

Class I mixture model (single-phase):

total mass	$\partial_t \rho + \mathrm{div}\,(\rho \mathbf{u}) = 0$
momentum	$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S}$
species mass	$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\,\mathbf{j}_i = 0$

with mass fractions $y_i = \rho_i / \rho$

Constitutive equations for multicomponent diffusive fluxes ?

Multicomponent single-phase fluid mixture

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Constitutive equations for multicomponent diffusive fluxes ?

Multicomponent single-phase fluid mixture

individual momentum balances in dimensionless form:

$$\partial_t(\rho_i^* \mathbf{u}_i^*) + \nabla \cdot (\rho_i^* \mathbf{u}_i^* \otimes \mathbf{u}_i^*) = -\mathrm{Eu}\, \phi_i \nabla p^* + \frac{1}{\mathrm{Re}} \nabla \cdot \mathbf{S}_i^*$$
$$- \mathrm{MS}\, c_{\mathrm{tot}}^* \Big(x_i \nabla_{T,p} \mu_i^* + \mathrm{Pe} \sum_{j \neq i} \frac{x_i\, x_j}{Đ_{ij}^*} (\mathbf{u}_i^* - \mathbf{u}_j^*) \Big)$$

with $Đ_{ij}^* = Đ_{ij}/Đ_0$, $\quad Đ_{ij} = 1/f_{ij}$ the *Maxwell-Stefan diffusivities* and ϕ_i the volume fractions.

$$\mathrm{Eu} = \frac{p_0}{\rho_0 U^2} \ \text{(Euler number)}, \qquad \mathrm{Re} = \frac{\rho_0\, U\, L}{\eta_0} \ \text{(Reynolds number)}$$
$$\mathrm{Pe} = \frac{U\, L}{Đ_0} \ \text{(Péclet number)}, \qquad \mathrm{MS} = \frac{c_0 R T}{\rho_0 U^2}$$

typical in applications: $\mathrm{MS} \approx 10^5$

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Multicomponent single-phase fluid mixture

requires, in the limit as $\mathrm{MS} \to \infty$:

$$\Big(x_i \nabla_{T,p} \mu_i^* + \mathrm{Pe} \sum_{j \neq i} \frac{x_i\, x_j}{Đ_{ij}^*} (\mathbf{u}_i^* - \mathbf{u}_j^*)\Big) = 0,$$

or, translated back to dimensional quantities:

$$\frac{x_i}{RT} \nabla_{T,p} \mu_i + \sum_{j \neq i} \frac{x_i\, x_j}{Đ_{ij}} (\mathbf{u}_i - \mathbf{u}_j) = 0$$

But pressure diffusion may not be negligible: $\frac{\mathrm{Eu}}{\mathrm{MS}} \not\approx 0$!
($\mathrm{Eu} \approx 100$ for atmospheric pressure)

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Note: $-\nabla p$ accelerates the full mixture!

$-\frac{\nabla p}{\rho}$ force per mass, hence $-y_i \nabla p$ is the part of the total pressure leading to the acceleration of species i as part of the full mixture.

Multicomponent single-phase fluid mixture

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$$-\,\mathrm{MS}\, c_{\mathrm{tot}}^* \Big(x_i \nabla_{T,p} \mu_i^* + \frac{\mathrm{Eu}}{\mathrm{MS}} \frac{\phi_i - y_i}{c_{\mathrm{tot}}^*} \nabla p^* + \mathrm{Pe} \sum_{j \neq i} \frac{x_i\, x_j}{Đ_{ij}^*} (\mathbf{u}_i^* - \mathbf{u}_j^*) \Big)$$

Define the molecular fluxes such that $(\ldots) = 0$, i.e.

$$\frac{x_i}{RT} \nabla_{T,p} \mu_i + (\phi_i - y_i) \frac{\nabla p}{c^{\mathrm{tot}} RT} + \sum_{j \neq i} \frac{x_j\, \mathbf{J}_i - x_i\, \mathbf{J}_j}{c^{\mathrm{tot}}\, Đ_{ij}} = 0$$

with $\mathbf{J}_i = c_i(\mathbf{u}_i - \mathbf{u}) = \mathbf{j}_i / M_i$

Generalized driving forces: $\mathbf{d}_i = \frac{x_i}{RT}\big(\nabla_T \mu_i - M_i \frac{\nabla p}{\rho}\big)$. Note: $\sum_i \mathbf{d}_i = 0$.

$$\mathbf{d}_i + \sum_{j \neq i} \frac{x_j\, \mathbf{J}_i - x_i\, \mathbf{J}_j}{c^{\mathrm{tot}}\, Đ_{ij}} = 0, \qquad \sum_i M_i \mathbf{J}_i = 0.$$

Multicomponent single-phase fluid mixture

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$$-\mathrm{MS}\, c_{\mathrm{tot}}^* \Big(x_i \nabla_{T,p} \mu_i^* + \frac{\mathrm{Eu}}{\mathrm{MS}} \frac{\phi_i - y_i}{c_{\mathrm{tot}}^*} \nabla p^* + \mathrm{Pe} \sum_{j \neq i} \frac{x_i\, x_j}{Đ_{ij}^*} (\mathbf{u}_i^* - \mathbf{u}_j^*) \Big)$$

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Multicomponent single-phase fluid mixture

single-phase fluid mixture with Maxwell-Stefan diffusion:

total mass	$\partial_t \rho + \mathrm{div}\,(\rho \mathbf{u}) = 0$
momentum	$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S}$
species mass	$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\,\mathbf{j}_i = 0$
diffusive fluxes	$\hat{\mathbf{d}}_i = -\sum_{j \neq i} \frac{y_j\,\mathbf{j}_i - y_i\,\mathbf{j}_j}{\rho \hat{Đ}_{ij}}, \quad \sum_i \mathbf{j}_i = 0$

mass based notations: $\hat{\mathbf{d}}_i = \frac{y_i}{RT}\left(\nabla_T \hat{\mu}_i - \frac{\nabla p}{\rho}\right)$ with $\hat{\mu}_i = \mu_i / M_i$,

$$\hat{Đ}_{ij} = M_i M_j Đ_{ij}$$

Multicomponent two-phase fluid mixtures

chemical components $A_1, \ldots, A_n$, partially miscible, no adsorption

individual mass balances:

$$\partial_t \rho_i + \mathrm{div}\,(\rho_i \mathbf{u}_i) = R_i \quad \text{in } \Omega \setminus \Gamma, \quad [\![\rho_i(\mathbf{u}_i - \mathbf{u}_\Gamma)]\!]\mathbf{n}_\Gamma = 0 \quad \text{on } \Gamma$$

$$\rho := \textstyle\sum_i \rho_i, \;\; \rho\mathbf{u} := \sum_i \rho_i \mathbf{u}_i, \;\; j = \rho(\mathbf{u} - \mathbf{u}_\Gamma) \cdot \mathbf{n}_\Gamma; \quad \sum_i R_i = 0$$

Continuity equation:

$$\partial_t \rho + \mathrm{div}\,(\rho\mathbf{u}) = 0 \quad \text{in } \Omega \setminus \Gamma, \quad [\![j]\!] = 0 \quad \text{on } \Gamma$$

Species equations:

$$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\,\mathbf{J}_i = 0 \quad \text{in } \Omega \setminus \Gamma,$$

$$[\![y_i]\!]\, j + [\![\mathbf{J}_i]\!]\mathbf{n}_\Gamma = 0 \quad \text{on } \Gamma$$

Multicomponent two-phase fluid mixtures

isothermal two-phase balances:

bulk	interface
$\partial_t \rho + \mathrm{div}\,(\rho \mathbf{u}) = 0$	$[\![\mathbf{u}]\!] = [\![\frac{1}{\rho}]\!]\, j \mathbf{n}_\Gamma$
$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S}$	$[\![\mathbf{u}]\!]\, j - [\![\mathbf{T}]\!] \cdot \mathbf{n}_\Gamma = \sigma \kappa \mathbf{n}_\Gamma$
	$V_\Gamma = \mathbf{u} \cdot \mathbf{n}_\Gamma + j/\rho$
$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\, \mathbf{j}_i = 0$	$[\![y_i]\!]\, j + [\![\mathbf{j}_i]\!] \mathbf{n}_\Gamma = 0$

One more constitutive relation at the interface is missing!

Energy dissipation (isothermal case)

total free energy:

$$E = \int_\Omega \rho\big(\tfrac{1}{2}|\mathbf{u}|^2 + \psi\big)\, dx + \int_\Gamma \sigma\, do$$

with $\rho\psi(\theta, \rho_1, \ldots, \rho_n)$ the free (available) energy density.

Euler relation:

$\rho\psi + p = \sum_i \hat{\mu}_i \rho_i$ with chemical potentials $\hat{\mu}_i = \partial_{\rho_i}(\rho\psi)$

energy dissipation:

$$\partial_t E = \int_\Omega \big(-\mathbf{S} : \nabla \mathbf{u} + p \operatorname{div} \mathbf{u} + \sum_i \nabla \hat{\mu}_i \cdot \mathbf{j}_i \big)\, dx$$

$$+ \int_\Gamma j\big([\![\frac{1}{2\rho^2}]\!] j^2 - [\![\mathbf{n}_\Gamma \cdot \mathbf{S}\mathbf{n}_\Gamma / \rho]\!]\big)\, do + \int_\Gamma \sum_i [\![\hat{\mu}_i]\!]\, j_i\, do$$

with $j_i := \rho_i(\mathbf{u}_i - \mathbf{u}_\Gamma) \cdot \mathbf{n}_\Gamma = j\, y_i + \mathbf{j}_i \cdot \mathbf{n}_\Gamma$; note that $[\![j_i]\!] = 0$.

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Chemical interface conditions

assumption: no interfacial energy dissipation

$$\Big([\![\tfrac{1}{2\rho^2}]\!]\, j^2 - [\![\mathbf{n}_\Gamma \cdot \mathbf{S}\mathbf{n}_\Gamma/\rho]\!] + [\![\hat{\mu}_1]\!]\Big)\, j + \sum_{i\neq 1}[\![\hat{\mu}_i - \hat{\mu}_1]\!]\, j_i = 0$$

chemical interface conditions:

$$[\![\hat{\mu}_i]\!] = [\![\mathbf{n}_\Gamma \cdot \mathbf{S}\mathbf{n}_\Gamma/\rho]\!] - [\![\tfrac{1}{2\rho^2}]\!]\, j^2 \quad \text{for all } i$$

note:

- the standard assumption in literature is $[\![\hat{\mu}_i]\!] = 0$ for all i
- consistency with the second law also requires $\mathbf{S} : \nabla \mathbf{u} \geq 0$ and $\sum_i \nabla\hat{\mu}_i \cdot \mathbf{j}_i \leq 0$

related models: D. Bedeaux, Advance in Chemical Physics LXIV (1986),
W. Dreyer, WIAS preprint No. 869 (2003).

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$$\left([\![\tfrac{1}{2\rho^2}]\!]\, j^2 - [\![\mathbf{n}_\Gamma \cdot \mathbf{S}\mathbf{n}_\Gamma/\rho]\!] + [\![\hat{\mu}_1]\!]\right) j + \sum_{i\neq 1} [\![\hat{\mu}_i - \hat{\mu}_1]\!]\, j_i = 0$$

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Multicomponent two-phase Navier-Stokes system

the full model:

bulk	interface
$\partial_t \rho + \mathrm{div}\,(\rho \mathbf{u}) = 0$	$[\![\mathbf{u}]\!] = [\![\frac{1}{\rho}]\!]\, j \mathbf{n}_\Gamma$
$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \mathbf{T}$	$[\![\mathbf{u}]\!]\, j - [\![\mathbf{T}]\!] \cdot \mathbf{n}_\Gamma = \sigma \kappa \mathbf{n}_\Gamma$
	$V_\Gamma = \mathbf{u} \cdot \mathbf{n}_\Gamma + j/\rho$
$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\, \mathbf{j}_i = 0$	$[\![y_i]\!]\, j + [\![\mathbf{j}_i]\!] \mathbf{n}_\Gamma = 0$
$\hat{\mathbf{d}}_i = -\sum_{j \neq i} \frac{y_j \mathbf{j}_i - y_i \mathbf{j}_j}{\rho \hat{Đ}_{ij}}, \; \sum_i \mathbf{j}_i = 0$	$[\![\hat{\mu}_i]\!] = [\![\mathbf{n}_\Gamma \cdot \mathbf{S} \mathbf{n}_\Gamma / \rho]\!] - [\![\frac{1}{2\rho^2}]\!]\, j^2$

Note: an incompressible version with $\rho_\pm \equiv const_\pm$ is also consistent.

The Fluxes

Inversion of the MS-equations on $E = \{u \in \mathbb{R}^n : \sum_i u_i = 0\}$:

$$[\mathbf{J}_i] = X^{\frac{1}{2}} (A_{S|E})^{-1} X^{-\frac{1}{2}} \, [\mathbf{d}_i] = \frac{1}{RT} X^{\frac{1}{2}} (A_{S|E})^{-1} X^{\frac{1}{2}} \, [\nabla \mu_i] \, .$$

Here $A_S := X^{-\frac{1}{2}} \, A \, X^{\frac{1}{2}}$ with $X = \mathrm{diag}(x_1, \ldots, x_n)$ and

$$A = \begin{bmatrix} -s_1 & & & d_{ij} \\ & \cdot & & \\ & & \cdot & \\ d_{ij} & & & -s_n \end{bmatrix}, \quad s_i = \sum_{k \neq i} \frac{x_k}{Đ_{ik}}, \quad d_{ij} = \frac{x_i}{Đ_{ij}}$$

is symmetric with $\sigma(A_{S|E}) \subset (-\infty, -\delta]$ for $\delta = \min\{1/Đ_{ij} : i \neq j\}$.

- $[\mathbf{J}_i] : [\nabla \mu_i] = \frac{1}{RT} \Big((A_{S|E})^{-1} X^{\frac{1}{2}} \, [\nabla \mu_i] \Big) : \Big(X^{\frac{1}{2}} \, [\nabla \mu_i] \Big) \leq 0.$
- $\mathrm{div}\,([\mathbf{J}_i]) =: \mathrm{div}\,(-\mathbf{D}(\mathbf{c}) \nabla \mathbf{c})$ has elliptic principal part if $\rho\psi$ is strongly convex

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$$[\mathbf{J}_i] = X^{\frac{1}{2}}(A_{S|E})^{-1} X^{-\frac{1}{2}} [\mathbf{d}_i] = \frac{1}{RT} X^{\frac{1}{2}}(A_{S|E})^{-1} X^{\frac{1}{2}} [\nabla \mu_i] .$$

Here $A_S := X^{-\frac{1}{2}} A X^{\frac{1}{2}}$ with $X = \mathrm{diag}(x_1, \ldots, x_n)$ and

$$A = \begin{bmatrix} -s_1 & & & d_{ij} \\ & \cdot & & \\ & & \cdot & \\ d_{ij} & & & -s_n \end{bmatrix}, \quad s_i = \sum_{k \neq i} \frac{x_k}{Đ_{ik}}, \quad d_{ij} = \frac{x_i}{Đ_{ij}}$$

is symmetric with $\sigma(A_{S|E}) \subset (-\infty, -\delta]$ for $\delta = \min\{1/Đ_{ij} : i \neq j\}$.

- $[\mathbf{J}_i] : [\nabla \mu_i] = \frac{1}{RT} \Big((A_{S|E})^{-1} X^{\frac{1}{2}} [\nabla \mu_i] \Big) : \Big(X^{\frac{1}{2}} [\nabla \mu_i] \Big) \leq 0.$
- $\mathrm{div}\,([\mathbf{J}_i]) =: \mathrm{div}\,(-\mathbf{D}(\mathbf{c})\nabla \mathbf{c})$ has elliptic principal part if $\rho\psi$ is strongly convex

Isothermal isobaric single-phase case

Theorem

Let $\Omega \subset \mathbb{R}^N$ *be open bounded with smooth* $\partial\Omega$. *Let* $p > \frac{N+2}{2}$ *and* $\mathbf{c}_0 \in W_p^{2-\frac{2}{p}}(\Omega)$ *such that* $c_i^0 > 0$ *in* $\bar{\Omega}$ *and* c_0^{tot} *is constant in* Ω. *Let the diffusion matrix* $\mathbf{D}(\mathbf{c})$ *be given by*

$$\mathbf{D}(\mathbf{c}) = X^{\frac{1}{2}}(A_{S|E})^{-1}X^{\frac{1}{2}}G''(\mathbf{x}) \ \ \textit{with}\ \mathbf{x} = \mathbf{c}/c^{\mathrm{tot}}, X = \mathrm{diag}(\mathbf{x}),$$

where $G := \rho\psi$ *is smooth and strongly convex on* $\{c^{\mathrm{tot}} = c_0^{\mathrm{tot}}\}$. *Then there exists - locally in time - a unique strong solution (in the* L^p*-sense) of*

$$\partial_t \mathbf{c} + \mathrm{div}\,(-\mathbf{D}(\mathbf{c})\nabla\mathbf{c}) = 0, \qquad \partial_\nu \mathbf{c}_{|\partial\Omega} = 0, \quad \mathbf{c}_{|t=0} = \mathbf{c}_0$$

This solution is in fact classical.

Isothermal isobaric single-phase case

Idea of proof: Let u be given by $c_{\rm tot} x_i = u_i + c^0_{\rm tot}/n$.

- evolution for u lives in $E = \{u \in \mathbb{R}^n : \sum_i u_i = 0\}$
- $\operatorname{div}(-\mathbf{D}(u)\nabla u) = \mathbf{D}(u)\,(-\Delta u) \;+$ lower order terms
- $\lambda \in \mathbb{C}$ and $v \in E$ with $\mathbf{D}(u)\,v = \lambda v$ means

$$X^{\frac{1}{2}}(A_{S|E})^{-1} X^{\frac{1}{2}} G''(\mathbf{x})\,v = \lambda v.$$

$$\Rightarrow \; \langle (A_{S|E})^{-1} X^{\frac{1}{2}} G''(\mathbf{x})\,v, X^{\frac{1}{2}} G''(\mathbf{x})\,v\rangle = \lambda \langle v, G''(\mathbf{x})\,v\rangle.$$

- left-hand side > 0 and $\langle v, G''(\mathbf{x})\,v\rangle > 0$ by assumption on G, hence $\lambda > 0 \;\Rightarrow\; \sigma(\mathbf{D}(u)) \subset (0,\infty)$ in $\mathcal{L}(E;E)$.

Solutions stay non-negative because of the structure of diffusive fluxes:

$$\mathbf{J}_i(\mathbf{c}) = -D_i(\mathbf{c})\,\mathrm{grad}\, c_i + c_i\,\mathbf{F}_i(\mathbf{c}, \nabla \mathbf{c}).$$

Isothermal isobaric single-phase case

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Solutions stay non-negative because of the structure of diffusive fluxes:

$$\boxed{\mathbf{J}_i(\mathbf{c}) = -D_i(\mathbf{c})\, \operatorname{grad} c_i + c_i\, \mathbf{F}_i(\mathbf{c}, \nabla \mathbf{c}).}$$

Multicomponent two-phase Navier-Stokes system

the full model:

bulk	interface
$\partial_t \rho + \mathrm{div}\,(\rho \mathbf{u}) = 0$	$[\![\mathbf{u}]\!] = [\![\frac{1}{\rho}]\!]\, j \mathbf{n}_\Gamma$
$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \mathbf{T}$	$[\![\mathbf{u}]\!]\, j - [\![\mathbf{T}]\!] \cdot \mathbf{n}_\Gamma = \sigma \kappa \mathbf{n}_\Gamma$
	$V_\Gamma = \mathbf{u} \cdot \mathbf{n}_\Gamma + j/\rho$
$\rho(\partial_t y_i + \mathbf{u} \cdot \nabla y_i) + \mathrm{div}\,\mathbf{j}_i = 0$	$[\![y_i]\!]\, j + [\![\mathbf{j}_i]\!] \mathbf{n}_\Gamma = 0$
$\hat{\mathbf{d}}_i = -\sum_{j \neq i} \frac{y_j \mathbf{j}_i - y_i \mathbf{j}_j}{\rho \hat{\mathrm{D}}_{ij}}, \ \sum_i \mathbf{j}_i = 0$	$[\![\hat{\mu}_i]\!] = [\![\mathbf{n}_\Gamma \cdot \mathbf{S} \mathbf{n}_\Gamma / \rho]\!] - [\![\frac{1}{2\rho^2}]\!]\, j^2$

We focus on the incompressible version with constant total densities $\rho_\pm \equiv const_\pm$.

Two-Phase Navier-Stokes-Maxwell-Stefan system

work in progress

- in the case Γ is a graph over $\mathbb{R}^{N-1}$, the Lopatinski-Shapiro conditions are satisfied in the isobaric case.

Hence, in the isobaric case the associated linear system with planar interface has maximal L_p-regularity.

- next step: check whether the Maxwell-Stefan multicomponent diffusion system is normally elliptic in the non-isobaric case.

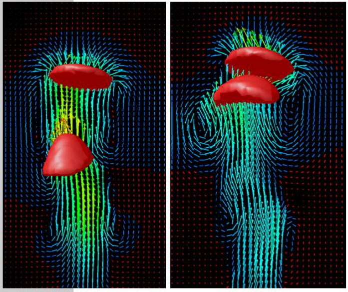
Volume of Fluid (VOF)-Method

- Direct Numerical Simulation of Navier-Stokes equations for two-phase flows
- implicit representation of interface : volume tracking, fractional volume f of dispersed phase
- additional advection equation for f

$$\partial_t f + \mathbf{u} \cdot \nabla f = 0$$

- piecewise linear interface reconstruction
- surface tension: conservative model
- massively parallelized
- well validated for collision of drops

Rieber, Frohn, *ITLR Stuttgart*



0	0	0	0	0
0.87	0.52	0.08	0	0
1	1	0.53	0	0
1	1	0.95	0	0

VOF-based Mass-Transfer Computation

mass balance in terms of molar concentration c_i:

$$\partial_t c_i + \nabla \cdot c_i \mathbf{u} + \nabla \cdot \mathbf{J}_i = r_i \qquad [\![c_i (\mathbf{u} - \mathbf{u}_\Gamma) + \mathbf{J}_i]\!] \cdot \mathbf{n}_\Gamma = 0$$

- molecular fluxes according to Fick´s law $\mathbf{J}_i^{\,j} = -D_i^j \nabla c_i^j, \quad j = L, G$
- no phase change: $[\![c_i (\mathbf{u} - \mathbf{u}_\Gamma)]\!] \cdot \mathbf{n}_\Gamma = \mathbf{0}, \quad \mathbf{J}_i^{\,L} \cdot \mathbf{n}_\Gamma = \mathbf{J}_i^{\,G} \cdot \mathbf{n}_\Gamma$
- local chemical equilibrium: $\mu_i^G = \mu_i^L$

$$\mu_i = \mu_i^0 + RT \ln a_i$$

a_i activity

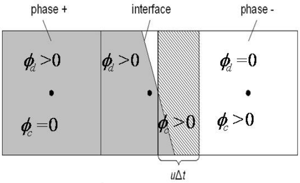
$a_i = \gamma_i c_i$

Henry´s law: $\dfrac{c_i^G}{c_i^L} = H_i$

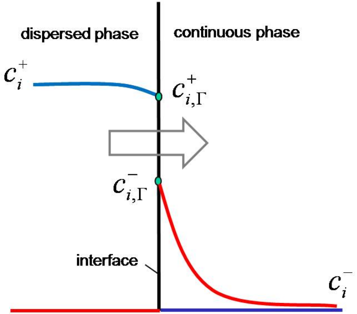
Two-Variable Mass-Transfer Approach

Problem: discontinuous species concentrations

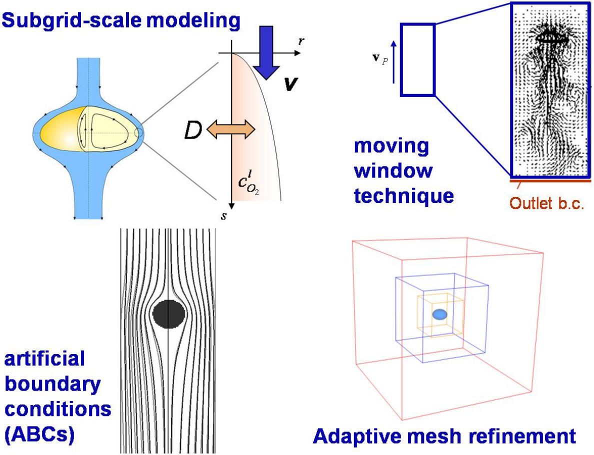
- two scalar quantities per species
- convective transport interlinked with VOF-transport using geometrically computed fluxes



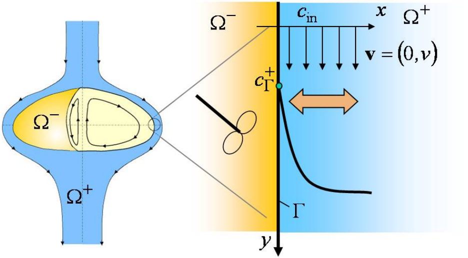
⇨ no artificial mass transfer



Enhancing the Interfacial Resolution



Subgrid-Scale Modeling

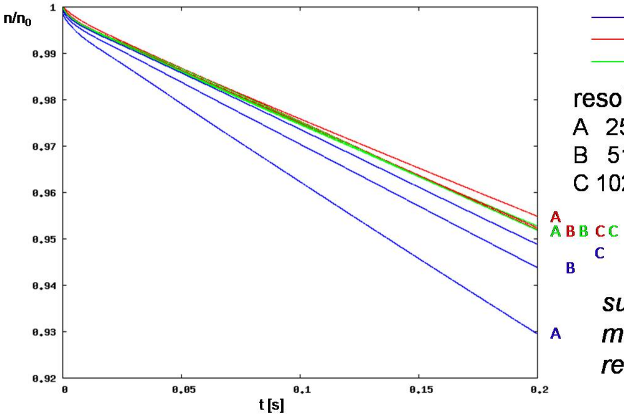


$$\partial_t c + \mathbf{v} \cdot \nabla c = D\,\Delta c$$
$$t > 0,\ x > 0,\ y > 0$$

$$c_{|y=0} = c_{\text{in}}$$
$$c_{|x=0} = c_\Gamma^+$$
$$c_{|x=\infty} = 0$$

$$c(x, y) = c_\Gamma^+ \left(1 - erf\left(\frac{x}{d(y)} \right) \right)$$

Effect of Subgrid-Scale Model



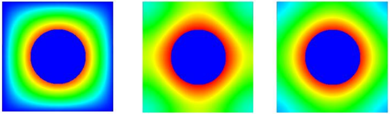
Evolution of species mass inside a rising 3 mm Blase, 2D, Sc = 10

- equilibrium
- linear gradient
- subgrid scale model

resolution:
A 256 x 128 cells
B 512 x 256 cells
C 1024 x 512 cells

subgrid-scale model saves one refinement level

Artificial Boundary Condition



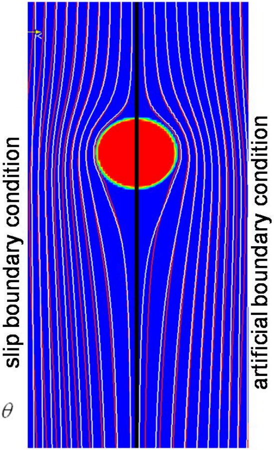
Dirichlet-BC Neumann-BC Robin-type BC

Hadamard-Rybczynski

$$u_r = \left(\frac{a_1}{r^3} + \frac{a_2}{r} - u_p \right) \cos\theta$$

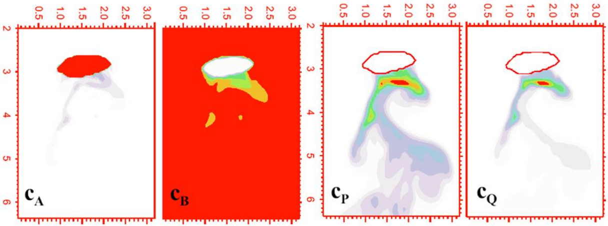
$$u_\theta = \left(\frac{1}{2}\frac{a_1}{r^3} - \frac{1}{2}\frac{a_2}{r} + u_p \right) \sin\theta$$

$$\frac{\partial u_r}{\partial r} + \frac{1}{r} u_r \approx -\frac{u_p}{r} cos\,\theta \qquad \frac{\partial u_\theta}{\partial r} + \frac{1}{r} u_\theta \approx \frac{u_p}{r} sin\,\theta$$



Mass Transfer with Chemical Reaction

$$A_g \rightarrow A_l \qquad A_l + B \xrightarrow{k_1} P \qquad A_l + P \xrightarrow{k_2} Q$$



3D VOF-simulation

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Many thanks to You for Your attention !