# Diffusion in multicomponent systems: from Maxwell-Stefan to compressible fluid models

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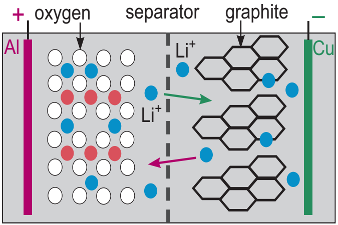
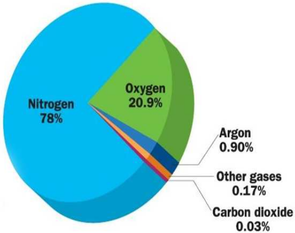


# Multicomponent systems

Most fluid systems in nature are composed of multiple components

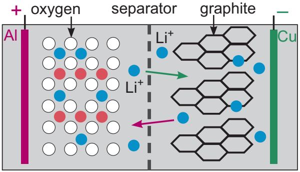
## Heliox:

- Air: 78% nitrogen, 21% oxygen
- Heliox: 79% helium, 21% oxygen
- Speeds up oxygen transport within bronchial tree
- Used in respiratory medicine (asthma), deep diving, and for coronavirus OC43 infection




## Lithium-ion batteries:

- Lithium$^+$ ions move from negative to positive electrode, electrons$^-$ flow through external circuit
- Electrolyte = mixture of organic carbonates



# Fick's law for mixtures

- Mass balance equations: densities $\rho_i$, diffusion fluxes $J_i$

$$\partial_t \rho_i + \operatorname{div} J_i = 0, \quad i = 1, \ldots, n$$

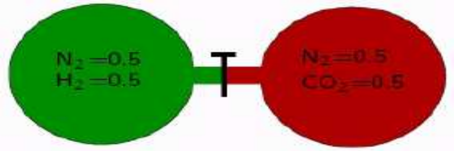
- Fick's law: flux from high-concentration to low-concentration region

$$J_i = -D_i \nabla \rho_i, \quad D_i : \text{ diffusion coefficient}$$

- Leads to diffusion equation $\partial_t \rho_i - \operatorname{div}(D_i \nabla \rho_i) = 0$

Problem: uphill diffusion in ternary mixtures (Duncan-Toor 1962)

- Mixture of hydrogen, nitrogen, carbon dioxide in two bulbs
- Flux of nitrogen $J_2$ significant although $\nabla \rho_2 \approx 0 \to$ uphill diffusion
- Friction forces between different species need to be taken into account



# Cross-diffusion

- Fick's law generally not valid for fluid mixtures
- Multicomponent diffusion:

$$\partial_t \rho_i + \operatorname{div} J_i = 0, \quad J_i = -\sum_{j=1}^{n} D_{ij} \nabla \rho_j$$

- Properties: $(D_{ij})$ symmetric (Onsager relation), positive semidefinite (second law of thermodynamics) $\to$ guarantees parabolicity of system
- Problem: $D_{ij} < 0$ possible, how to prove that $\rho_i \geq 0$?
- Recall Fick's ansatz: $\nabla \rho_i = J_i = \rho_i v_i$ ($v_i$: velocity, ideal gas), i.e. driving force proportional to velocity
- Ansatz: driving force = friction force = proportional to relative velocity $v_j - v_i$ leads to Maxwell-Stefan equations

$$\partial_t \rho_i + \operatorname{div}(\rho_i v_i) = 0, \quad \nabla \rho_i = \sum_{j=1}^{n} C_{ij} \rho_i \rho_j (v_j - v_i)$$

- Incompressibility cond.: $\sum_{i=1}^{n} \rho_i = 1$ (consequence of $\sum_{i=1}^{n} \rho_i v_i = 0$)

# Model hierarchy for fluid mixtures

- Isothermal diffusive fluid: Maxwell-Stefan equations

$$\partial_t \rho_i + \operatorname{div} J_i = r_i(\rho), \quad \text{relation between } J_i \text{ and } \nabla \rho_j$$

- Heat-conducting diffusive fluid: add energy equation

$$\partial_t \rho_i + \operatorname{div} J_i = r_i(\rho), \quad \partial_t(\rho_{\rm tot} E) + \operatorname{div} Q = 0$$

$$E: \text{ total energy}, \quad Q: \text{ heat flux}, \quad \rho_{\rm tot} = \textstyle\sum_{i=1}^n \rho_i$$

- Isothermal compressible fluid: add Euler or Navier-Stokes eqs.

$$\partial_t \rho_i + \operatorname{div}(\rho_i v + J_i) = r_i(\rho), \quad v: \text{ fluid velocity}$$

$$\partial_t(\rho_{\rm tot} v) + \operatorname{div}(\rho_{\rm tot} v \otimes v + \bar{S}) = 0, \quad \bar{S}: \text{ stress tensor}$$

- Heat-conducting compressible fluid: Maxwell-Stefan-Navier-Stokes-Fourier

$$\partial_t \rho_i + \operatorname{div}(\rho_i v + J_i) = r_i(\rho)$$

$$\partial_t(\rho_{\rm tot} v) + \operatorname{div}(\rho_{\rm tot} v \otimes v + \bar{S}) = 0$$

$$\partial_t(\rho_{\rm tot} E) + \operatorname{div}(\rho_{\rm tot} E v - \bar{S} v + Q) = 0$$

# Overview

- Introduction
- Maxwell-Stefan equations
- Extensions
- Compressible fluid models

# Maxwell-Stefan equations

$$\partial_t \rho_i + \operatorname{div}(\rho_i v_i) = r_i(\rho), \quad \nabla \rho_i = \sum_{j=1}^{n} C_{ij} \rho_i \rho_j (v_j - v_i)$$

- Isobaric, isothermal, same molar masses, condition $\sum_{i=1}^{n} \rho_i = 1$
- Suggested by J. Maxwell (1866) and J. Stefan (1871)
- Derivation from Boltzmann equation if evolution close to equilibrium: Boudin-Grec-Salvarani 2015, Bondesan-Briant 2019
- Derivation from Euler equations: Huo-A.J.-Tzavaras 2019
- Thermodynamics: Giovangigli 1999, Bothe-Dreyer 2015

Mathematical analysis:

- Global existence of solutions around equil.: Giovangigli-Massot 1998
- Local existence of classical solutions: Bothe 2011
- Global existence of weak solutions: A.J.-Stelzer 2013
- $L^p$-maximal regularity: Herberg-Meyries-Prüss-Wilke 2017

# Mathematical difficulties

$$\partial_t \rho_i + \operatorname{div}(\rho_i v_i) = r_i(\rho), \quad \nabla \rho_i = \sum_{j=1}^n C_{ij}\rho_i\rho_j(v_j - v_i) =: (CJ)_i$$

- Aim: write equations as

$$\partial_t \rho_i - \operatorname{div} \sum_{j=1}^n M_{ij}(\rho)\nabla\rho_j = r_i(\rho), \quad i = 1, \ldots, n$$

- Problem: $\sum_{i=1}^n \rho_i = 1 \Rightarrow \sum_{i=1}^n \nabla\rho_i = 0 \Rightarrow \ker(C) = \operatorname{span}\{1\}$
- Solution: invert $C$ on $\operatorname{Im}(C) = \ker(C)^\perp$

$$\partial_t \rho - \operatorname{div}(A(\rho)\nabla\rho) = r(\rho), \quad A = C|_{\operatorname{Im}(C)}, \ \rho = (\rho_1, \ldots, \rho_n)$$

- $A$ neither symmetric nor positive definite, but eigenvalues of $A$ have positive real parts $\Rightarrow$ parabolic in the sense of Petrovskii
- Amann 1990: local-in-time existence of classical solutions
- Problem: global existence, proof of $0 \le \rho_i \le 1$
- Solution: exploit entropy structure

# Entropy structure

$$\partial_t \rho_i - \operatorname{div} \sum_{i=1}^{n} A_{ij}(\rho)\nabla \rho_j = r_i(\rho), \quad i = 1, \ldots, n$$

- Entropy density: $h(\rho^*) = \sum_{i=1}^n \rho_i(\log \rho_i - 1)$, $\rho_n = 1 - \sum_{i=1}^{n-1} \rho_i$
- Entropy variable: $w_i = \partial h / \partial \rho_i$, $\rho^* = (\rho_1, \ldots, \rho_{n-1})$

$$\partial_t \rho_i - \operatorname{div} \sum_{j=1}^{n-1} B_{ij}(w)\nabla w_j = r_i(\rho), \quad i = 1, \ldots, n-1$$

Benefits:

- Diffusion matrix $B(w) = A(\rho)h''(\rho^*)^{-1}$ positive (semi) definite
- Lower and upper bounds: $w_i = \log(\rho_i/\rho_n)$ can be inverted

$$\rho_i = \frac{e^{w_i}}{1 + \sum_{j=1}^{n-1} e^{w_j}} \in (0,1)$$

- A priori estimates from entropy production:

$$\frac{d}{dt}\int_\Omega h(\rho^*)dx + \kappa \int_\Omega \sum_{i=1}^{n-1} |\nabla \sqrt{\rho_i}|^2 dx \le \int_\Omega \sum_{i=1}^{n-1} r_i \cdot \frac{\partial h}{\partial \rho_i} dx \le 0$$

# Gradient-flow and thermodynamic structure

$$\partial_t \rho_i - \operatorname{div} \sum_{j=1}^{n-1} B_{ij}(w)\nabla w_j = 0, \quad i = 1, \dots, n-1$$

Gradient-flow structure: write equations as

$$\partial_t \rho_i - \operatorname{div}\left(\sum_{j=1}^{n-1} B_{ij}\nabla\frac{\delta H}{\delta \rho^*}\right) = 0, \quad w_i = \frac{\delta H}{\delta \rho_i}$$

- Entropy $H = \int_\Omega h(\rho^*)dx = \int_\Omega \sum_{i=1}^n \rho_i(\log\rho_i - 1)$
- Gradient flow: $\partial_t \rho = -K[\rho^*]\mathrm{grad} H|_\rho$ on differential manifold, where $K[\rho^*]w = -\operatorname{div}(B\nabla w)$ Onsager operator

Thermodynamic structure:

- Mathematical entropy density $h = -s$ physical entropy density
- Entropy variable = chemical potential $w_i = \partial h/\partial \rho_i$
- Onsager reciprocal relations: $B$ is symmetric
- Entropy production: $-\frac{dH}{dt} = \int_\Omega \nabla w : B\nabla w dx \geq 0$
  $\rightarrow$ expresses second law of thermodynamics

# Global existence of weak solutions

$$\partial_t \rho_i - \operatorname{div} \sum_{j=1}^n A_{ij} \nabla \rho_j = r_i(\rho) \quad \text{in } \Omega,\ t > 0,\ \rho_i(0) = \rho_i^0,\ \text{no-flux b.c.}$$

**Theorem (A.J.-Stelzer 2013)**

*Let* $\rho_i^0 \geq 0$, $\sum_{i=1}^n \rho_i^0 \leq 1$, $\sum_{i=1}^n r_i = 0$, $\sum_{i=1}^n r_i \log(\rho_i/\rho_n) \leq 0$. *Then* $\exists$ *weak solution* $\rho_i \in L^2(0,T;H^1(\Omega))$, $\partial_t \rho_i \in L^2(0,T;H^2(\Omega)')$, *and*

$$0 \leq \rho_1, \ldots, \rho_{n-1} \leq 1, \quad \rho_n = 1 - \textstyle\sum_{i=1}^{n-1} \rho_i \geq 0 \quad \text{in } \Omega,\ t > 0$$

Ideas of proof:

- Approximations: implicit Euler in time, higher-order regularization in space (important: preserves entropy structure)
- Fixed-point argument for approximated system: compactness comes from higher-order regularization term
- De-regularization limit: compactness comes from entropy estimate and nonlinear discrete Aubin-Lions lemma

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# Barycentric velocity (Huo-A.J.-Tzavaras 2019)

- Consider isothermal ideal fluid mixture described by Euler equations

$$\partial_t \rho_i + \operatorname{div}(\rho_i v_i) = 0, \quad i = 1, \ldots, n$$
$$\partial_t(\rho_i v_i) + \operatorname{div}(\rho_i v_i \otimes v_i) + \nabla p_i(\rho) = -\frac{1}{\varepsilon}\sum_{j=1}^n b_{ij}\rho_i\rho_j(v_i - v_j)$$

- Partial mass density $\rho_i$, partial velocity $v_i$, partial pressure $p_i(\rho)$
- Barycentric velocity $v = \rho_{\rm tot}^{-1}\sum_{i=1}^n \rho_i v_i$, $\rho_{\rm tot} = \sum_{i=1}^n \rho_i$
- Chapman-Enskog expansion: $\rho_i = \widehat{\rho}_i + O(\varepsilon^2)$, $v = \widehat{v} + O(\varepsilon^2)$
- $(\widehat{\rho}_i, \widehat{v})$ solve Maxwell-Stefan equations

$$\partial_t \widehat{\rho}_i + \operatorname{div}\left(\widehat{\rho}_i \widehat{v} - \varepsilon\sum_{j=1}^n \frac{b_{ij}}{\widehat{\rho}_j}\nabla p_j(\widehat{\rho})\right) = O(\varepsilon^2), \quad i = 1, \ldots, n$$
$$\partial_t(\widehat{\rho}_{\rm tot}\widehat{v}) + \operatorname{div}(\widehat{\rho}_{\rm tot}\widehat{v} \otimes \widehat{v}) + \sum_{i=1}^n \nabla p_i(\widehat{\rho}) = O(\varepsilon^2)$$

- Total mass density: $\widehat{\rho}_{\rm tot} = \sum_{i=1}^n \widehat{\rho}_i$
- Idea of proof: estimate $\rho_i - \widehat{\rho}_i$ from relative free energy

# Maxwell-Stefan with temperature (Helmer-A.J. 2020)

Maxwell-Stefan system can be written as

$$\partial_t \rho_i + \operatorname{div} J_i = r_i, \ \ J_i = -\sum_{j=1}^n M_{ij} \nabla w_j, \quad \ker(M_{ij}) = \operatorname{span}\{1\}$$

Include temperature $\theta$:

$$\partial_t \rho_i + \operatorname{div} J_i = r_i, \quad J_i = -\sum_{j=1}^n M_{ij}(\rho,\theta)\nabla q_j - M_i(\rho,\theta)\nabla\frac{1}{\theta}$$

$$\partial_t(\rho_{\text{tot}}\theta) + \operatorname{div} J_e = 0, \quad J_e = -\kappa(\theta)\nabla\theta - \sum_{j=1}^n M_j(\rho,\theta)\nabla q_j$$

- Thermo-chemical potentials: $q_i = w_i/\theta$, heat conductivity: $\kappa(\theta)$
- Properties: $\sum_{j=1}^n M_{ij} = 0$, $\sum_{i=1}^n M_i = 0$, $z^\top M z \geq c|\Pi z|^2$ for $z \in \mathbb{R}^n$

**Theorem (Helmer-A.J., in progress)**

*Let $\kappa(\theta) \leq c(1+\theta^p)$ with $p < 2/3$, $\sum_{i=1}^n r_i = 0$, $\sum_{i=1}^n r_i q_i \leq -c|\Pi q|^2$. Then $\exists$ weak solution $\rho_1,\ldots,\rho_n,\theta$ such that $0 \leq \rho_i \leq 1$.*

Idea of proof: $h = \rho_i(\log\rho_i - 1) - \rho_{\text{tot}}\log\theta$, $\rho_{\text{tot}}(t) = \rho_{\text{tot}}(0)$

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# Navier-Stokes equations

Aim: Couple Maxwell-Stefan with Navier-Stokes and heat flow

Incompressible Navier-Stokes equations:

$$\operatorname{div} v = 0, \quad \partial_t(\rho v) + \operatorname{div}(\rho v \otimes v) + \nabla p = \eta \Delta v + (\eta + \nu)\nabla(\operatorname{div} u)$$

- Existence theory for incompressible NSE: Leray 1934, Ladyzhenskaya 1969, Temam 1977, P.-L. Lions 1996
- Millennium problem: existence of smooth solutions in $\mathbb{R}^3$

Compressible Navier-Stokes equations (NSE):

$$\partial_t \rho + \operatorname{div}(\rho v) = 0, \; \partial_t(\rho v) + \operatorname{div}(\rho v \otimes v) + \nabla \rho^\gamma = \eta \Delta v + (\eta + \nu)\nabla(\operatorname{div} u)$$

- Existence theory for compressible NSE: P.-L. Lions 1998 for $\gamma > \frac{9}{5}$, Feireisl-Novotný-Petzeltová 2001 for $\gamma > \frac{3}{2}$
- Stationary compressible NSE for fluid mixtures: Zatorska 2011 with Fick's law and $\gamma > \frac{7}{3}$, Giovangigli-Pokorný-Zatorska 2015 with $\gamma > \frac{5}{3}$, Piasecki-Pokorný 2017 with $\gamma > 1$

# Navier-Stokes-Fourier equations for one species

- Mass balance equation: reaction term $r(\rho, \theta)$

$$\partial_t \rho + \mathrm{div}(\rho v) = r(\rho, \theta)$$

- Momentum balance equation: viscous stress tensor $S$

$$\partial_t(\rho v) + \mathrm{div}(\rho v \otimes v) + \nabla p(\rho, \theta) = \mathrm{div}\, S := \eta \Delta v + (\eta + \nu)\nabla(\mathrm{div}\, v)$$

- Energy equation: total energy $E = e + |v|^2/2$, temperature $\theta$

$$\partial(\rho E) + \mathrm{div}(\rho E v - S v + p v + Q) = 0, \quad Q = -\kappa(\theta)\nabla\theta$$

- Consequence: balance equations for entropy $s$

$$\partial_t(\rho_{\mathrm{tot}} s) + \mathrm{div}(\rho s v + \kappa(\theta)\nabla \log\theta) = \frac{1}{\theta} S : \nabla v + \kappa(\theta)|\nabla \log\theta|^2 \geq 0$$

- Existence results: P.-L. Lions 1998, Mucha-Pokorný 2010, Feireisl-Karper-Novotný 2016

Aim: extend model to mixtures

# Maxwell-Stefan-Navier-Stokes-Fourier equations

Balance equations: $\rho_{\mathrm{tot}} = \sum_{i=1}^n \rho_i$

$$\partial_t \rho_i + \operatorname{div}(\rho_i v + J_i) = r_i, \quad i = 1, \ldots, n$$
$$\partial_t(\rho_{\mathrm{tot}} v) + \operatorname{div}(\rho_{\mathrm{tot}} v \otimes v) + \nabla p(\rho, \theta) = \operatorname{div} S + \rho_{\mathrm{tot}} b$$
$$\partial_t(\rho_{\mathrm{tot}} E) + \operatorname{div}(\rho_{\mathrm{tot}} E v - S v + p v + Q) = \rho_{\mathrm{tot}} b \cdot v$$

Constitutive equations:

- Diffusion fluxes: $J_i = -\sum_{j=1}^n M_{ij}(\rho, \theta)\nabla(w_i/\theta) - M_i \nabla(1/\theta)$
- Viscous stress tensor: $S$ = function of $\nabla v$ and $\theta$
- Heat flux: $Q = -\kappa(\theta)\nabla\theta - \sum_{i=1}^n M_i \nabla(w_i/\theta)$, $w_i$: chem. potential

Option: replace energy balance with $E$ by entropy inequality:

$$\partial_t(\rho s) + \operatorname{div} J_S + P_S \geq 0 \quad \& \quad \text{integrated energy balance}$$

- Entropy flux: $J_S$ = contributions due to diffusion and heat fluxes
- Entropy production: $P_S$ = contributions due to diffusion, heat, viscous stress & reactions

# Maxwell-Stefan-Navier-Stokes-Fourier equations

Model equations: $\rho_{\rm tot} = \sum_{i=1}^n \rho_i$

$$\partial_t\rho_i + \operatorname{div}(\rho_i v + J_i(w)) = r_i, \quad i = 1,\ldots,n$$

$$\partial_t(\rho_{\rm tot} v) + \operatorname{div}(\rho_{\rm tot} v\otimes v) + \nabla p(\rho,\theta) = \operatorname{div} S + \rho_{\rm tot} b$$

$$\partial_t(\rho_{\rm tot} s) + \operatorname{div} J_S + P_S \ge 0 \quad \& \quad \text{integrated energy balance}$$

Variables determined from free energy: given $H = H(\rho,\theta)$

- Chemical potentials: $w_i = \partial H/\partial\rho_i$, $i = 1,\ldots,n$
- Pressure: $p(\rho,\theta) = -H + \sum_{i=1}^n \rho_i w_i$ (Gibbs-Duhem)
- (Physical) entropy density: $\rho_{\rm tot} s = -\partial H/\partial\theta$
- Total energy: $E = H - \theta\partial H/\partial\theta + |v|^2/2$

Boundary conditions:

- No-flux conditions for diffusion fluxes: $J_i\cdot\nu = 0$ on $\partial\Omega$
- Navier slip conditions for velocity: $v\cdot\nu = 0$, $\Pi_\perp(S\nu + v) = 0$ on $\partial\Omega$
- Robin conditions for temperature: $Q\cdot\nu + \alpha(\theta_0 - \theta) = 0$ on $\partial\Omega$

Goal: existence of stationary solutions in $\Omega\subset\mathbb{R}^3$

# Maxwell-Stefan-Navier-Stokes-Fourier equations

$$\operatorname{div}(\rho_i v + J_i) = r_i, \quad J_i = -\sum_{j=1}^n M_{ij}\nabla(w_i/\theta) - M_i\nabla(1/\theta)$$

$$\operatorname{div}(\rho_{\rm tot} v \otimes v) + \nabla p(\rho,\theta) = \operatorname{div} S + \rho_{\rm tot} b, \quad i = 1,\ldots,n$$

$$\operatorname{div} J_S + P_S \geq 0 \quad \& \quad \text{integrated energy balance}$$

Assumptions:

- Free energy: $H(\rho,\theta)$ strictly convex in $\rho$
- Diffusion matrix: $z^\top Mz \geq C|\Pi z|^2$, $\Pi$: projector on $\operatorname{span}\{1\}^\perp$
- Reactions: $\sum_{i=1}^n r_i = 0$ and $\sum_{i=1}^n r_i w_i/\theta \leq -C|\Pi(w/\theta)|^2$
- Pressure: $p(\rho,\theta)$ behaves like $\rho\theta + \rho^\gamma$ & other growth conditions

**Theorem (Buliček-A.J.-Pokorný-Zamponi 2020)**

*If $\gamma > 3/2$, $\exists$ renorm. variational entropy solution $(\rho_i, v, \theta)$, $\rho_i \in L^\gamma(\Omega)$*

- Solution concept: weak solution to above-mentioned equations and $\rho_{\rm tot}$ renormalized solution to continuity equation
- $\gamma > 1$ possible but stronger growth conditions (Novotný-Pokorný 2011)

# Ideas of proof

$$\operatorname{div}(\rho_i v + J_i) = r_i, \quad J_i = -\sum_{j=1}^n M_{ij}(\rho,\theta)\nabla(w_i/\theta) - M_i\nabla(1/\theta)$$

$$\operatorname{div}(\rho_{\rm tot} v \otimes v) + \nabla p(\rho,\theta) = \operatorname{div} S + \rho_{\rm tot} b, \quad i = 1,\dots,n$$

$$\operatorname{div} J_S + P_S \geq 0 \quad \& \quad \text{integrated energy balance}, \quad p(\rho,\theta) \sim \rho\theta + \rho^\gamma$$

- Six-level approximate problem: Galerkin approximation for velocity, lower-order and higher-order regularizations, regularization of the free energy give approximate solution $(\rho_i^\varepsilon, v^\varepsilon, \theta^\varepsilon)$
- Entropy balance: estimates for $|\nabla v^\varepsilon|^2$, $\nabla(w_i^\varepsilon/\theta^\varepsilon)$, $\log\theta^\varepsilon \Rightarrow \theta^\varepsilon > 0$
- Momentum balance and Bogovskii operator: estimate for $\rho_{\rm tot}^\varepsilon$ in $L^{\gamma+\nu}(\Omega)$ with $\nu > 0 \Rightarrow$ pressure $p^\varepsilon$ bounded in $L^\alpha(\Omega)$ for $\alpha > 1$
- Estimate effective viscous flux of Feireisl (measures oscillations of $\rho_i^\varepsilon$)
- Convexity of free energy: estimate $W_k = \overline{p^\varepsilon T_k(\rho_{\rm tot}^\varepsilon)} - \overline{p^\varepsilon}\,\overline{T_k(\rho_{\rm tot}^\varepsilon)}$, show that $W_k = 0$, conclude that $\rho_i^\varepsilon \to \rho_i$ in $L^1(\Omega)$ (new proof)

# Summary and perspectives

## Summary:

- Fick's law not sufficient in mixtures $\Rightarrow$ cross-diffusion
- Analysis of Maxwell-Stefan eqs.: method yields $L^\infty$ bounds without use of maximum principle (entropy method)
- Extensions: include barycentric velocity, temperature
- Compressible fluid mixtures: thermodynamical consistency important, new compactness proof for particle density

## Perspectives:

- Regularity of weak solutions to Maxwell-Stefan systems
- Stochastic Maxwell-Stefan systems: martingale solutions done (Dhariwahl-Huber-A.J.-Kuehn-Neamtu 2019); strong solutions?
- Time-dependent eqs. for compressible heat-conducting fluid mixtures

Key message: Thermodynamically consistent models for fluid mixtures very complex: combine entropy methods and math fluid dynamics tools