Multicomponent transport in plasmas; exploiting stoichiometry

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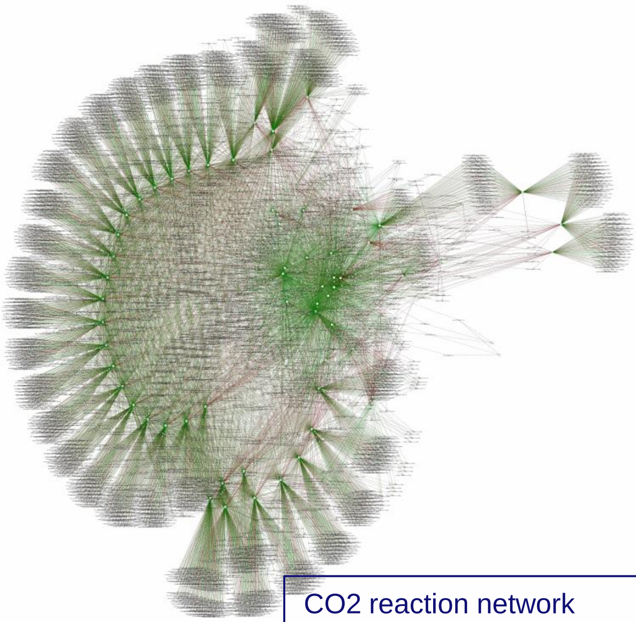
Where innovation starts

Multicomponent transport in plasmas

- **Rich chemistry**
- **CO_2: 72 components, 5732 reactions [1]**
- **Reaction components not independent**
- **Idea from porous media: Exploit relations between reactions [2]**
- **Here: Extend concept to plasmas**



CO2 reaction network

[1] Koelman, P. (2019). Chemical aspects of CO2 plasma modelling
[2] Krautle, Knabner (2007) A reduction scheme for the coupled multicomponent transport-reaction problems in porous media

Conservation laws

- **Generic conservation law:**

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \vec{\Gamma}_i = s_i$$

- **For clarity: steady state, 1D:**

$$\frac{d\Gamma_i}{dx} = s_i$$

Conservation laws

- **Fluxes via advection & Stefan-Maxwell diffusion**
- **Source-term generally non-linear**

$$\frac{d\Gamma_i}{dx} = s_i$$

- **Multicomponent: Coupled set**
  - **►Goal: simplify generic system**

Simple argon plasma

- **1 Reaction, 3 species**

$$\mathrm{Ar} \rightleftharpoons \mathrm{Ar}^{+} + \mathrm{e}^{-},$$

- **Coupled conservation laws**

$$\frac{d\Gamma_{Ar}}{dx} = s_{Ar}$$
$$\frac{d\Gamma_{Ar^{+}}}{dx} = s_{Ar^{+}}$$
$$\frac{d\Gamma_{e^{-}}}{dx} = s_{e^{-}}$$

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Simple argon plasma

- **1 Reaction, 3 species**

$$\mathrm{Ar} \rightleftharpoons \mathrm{Ar}^{+} + \mathrm{e}^{-},$$

- **Result: 3 Coupled conservation laws**
- **Stoichiometry: 2 constraints**
  - ► **Argon conservation** $s_{Ar} + s_{Ar^+} = 0$
  - ► **Charge conservation** $s_{Ar^+} - s_{e^-} = 0$

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Simple argon plasma

- **Idea: Exploit stoichiometry to simplify source-terms**
- **Linear combination of conservation laws**
- **Argon conservation**

$$\frac{d\Gamma_{Ar}}{dx} + \frac{d\Gamma_{Ar^+}}{dx} = s_{Ar} + s_{Ar^+} = 0$$

- **Charge conservation**

$$\frac{d\Gamma_{Ar^+}}{dx} - \frac{d\Gamma_{e^-}}{dx} = s_{Ar^+} - s_{e^-} = 0$$

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Simple argon plasma

- **Resulting transformed set**

$$\frac{d}{dx}\left(\Gamma_{Ar} + \Gamma_{Ar^+}\right) = 0$$

"Argon conserved"

$$\frac{d}{dx}\left(\Gamma_{Ar^+} - \Gamma_{e^-}\right) = 0$$

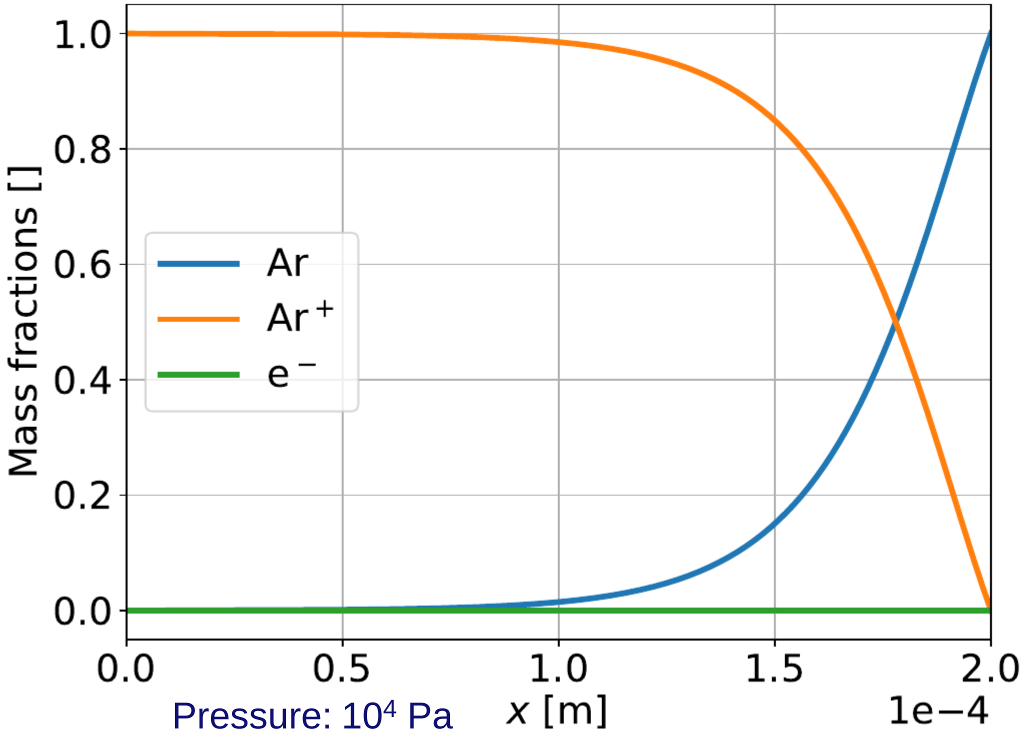
"Charge conserved"

$$\frac{d\Gamma_{e^-}}{dx} = s_{e^-}$$

"Leftover equation"

Argon system

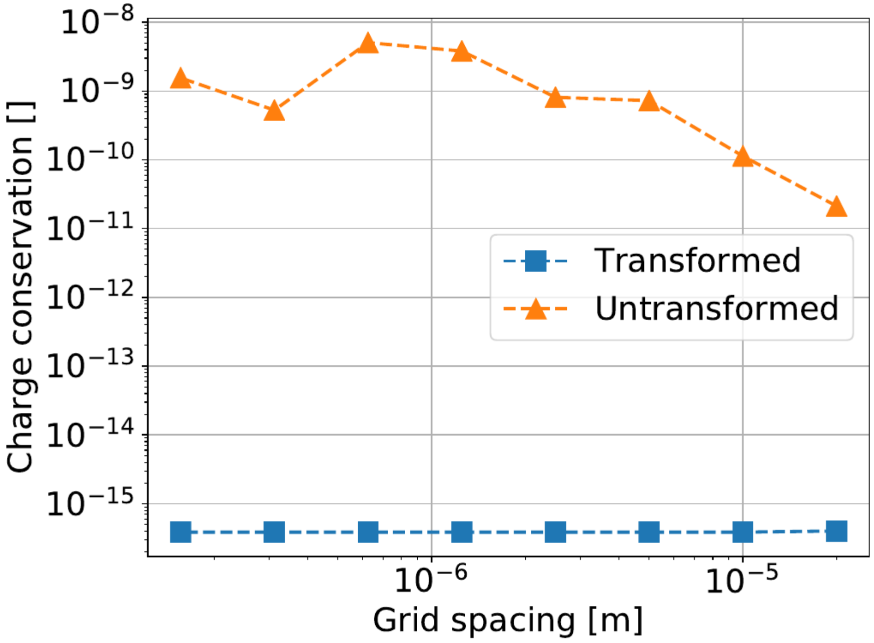
- **Dirichlet boundary conditions**
- **Central difference discretization**
- **Compare conservation original & transformed set**

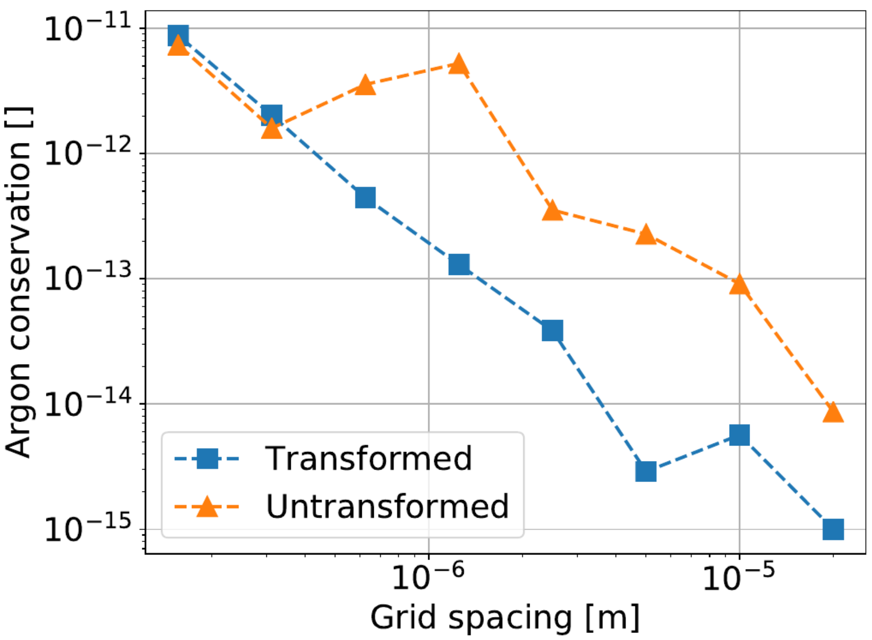


Pressure: 10^4 Pa
Temperature: 10^4 K
Mass flux: -20 kgm^{-2} s^{-1}

Charge – Argon conservation

- **Charge conservation much improved**
- **Argon conservation affected by rounding error**





Conclusion

- **Reaction properties used to transform system**
- **Transformed system partly source-free**
- **Numerically favorable properties for example system**

Outlook

- **Apply to complex chemistry**
- **Exploit source-free set**
- **Further optimize transformations**