Stoichiometric projection methods for plasma simulations

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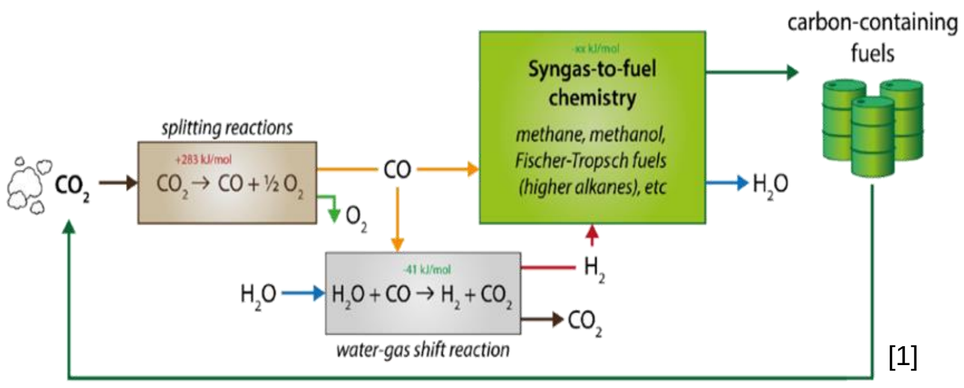
Introduction

Goal: CO_2 decomposition with plasmas for synthetic fuel processing

Numerical simulation challenge: >70 components, >5000 reactions[2]

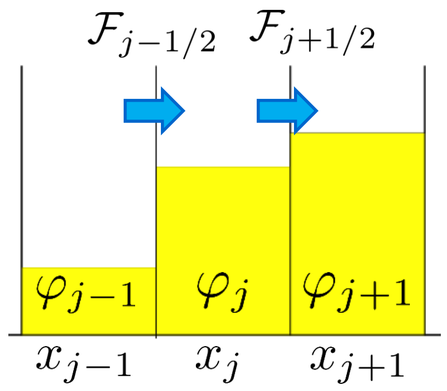


[1]

2. System of conservation laws

Drift-Diffusion-Reaction system (continuous)

$$\frac{d}{dx}\underbrace{\left(\boldsymbol{u}\varphi - \boldsymbol{\mathcal{E}}\frac{d\varphi}{dx}\right)}_{:=\mathcal{F}(\varphi)} = \boldsymbol{s}(\varphi)$$



Drift-Diffusion-Reaction system (discrete)

$$\mathcal{F}_{j+1/2} - \mathcal{F}_{j-1/2} = \Delta x \boldsymbol{s}(\boldsymbol{\varphi}_j)$$

3. Argon plasma test case

Stoichiometric projection: decouple system in conserved variables and others[3]

1 Reaction, 3 species

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

Stoichiometry: 2 constraints on sources

1.Charge conservation

$$s_{Ar^+} - s_{e^-} = 0$$

2. Argon conservation

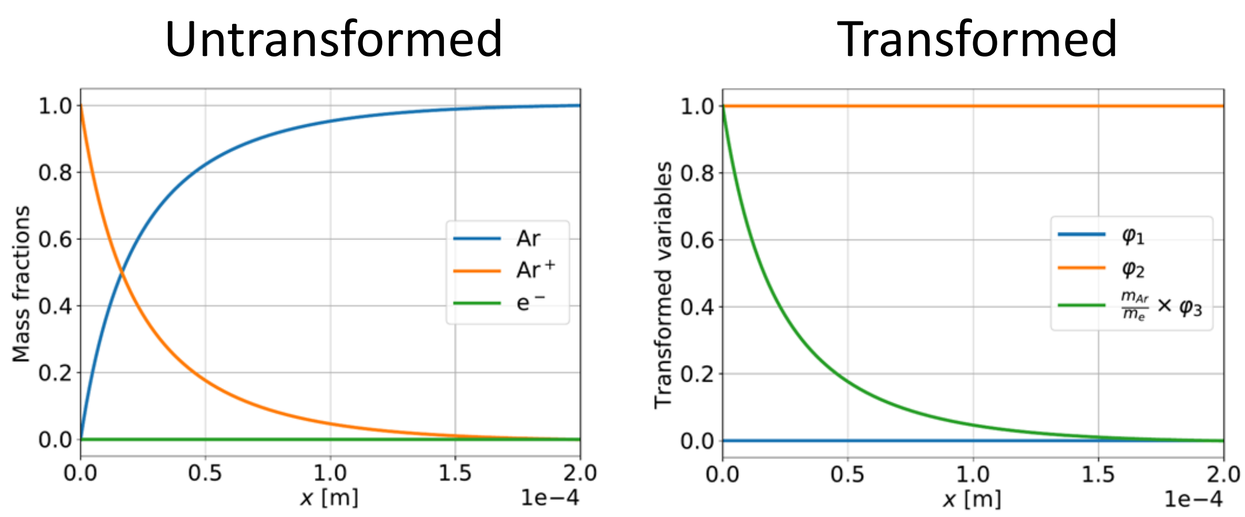
$$s_{Ar} + s_{Ar^+} = 0$$

Linear transformation of original equation set

$$\begin{aligned} \frac{d\mathcal{F}_{Ar}}{dx} &= s_{Ar} \\ \frac{d\mathcal{F}_{Ar^+}}{dx} &= s_{Ar^+} \\ \frac{d\mathcal{F}_{e^-}}{dx} &= s_{e^-} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \frac{d}{dx}\left(\mathcal{F}_{Ar^+} - \mathcal{F}_{e^-}\right) &= 0 \qquad \varphi_1 \\ \frac{d}{dx}\left(\mathcal{F}_{Ar} + \mathcal{F}_{Ar^+}\right) &= 0 \qquad \varphi_2 \\ \frac{d\mathcal{F}_{e^-}}{dx} &= s_{e^-} \qquad \varphi_3 \end{aligned}$$

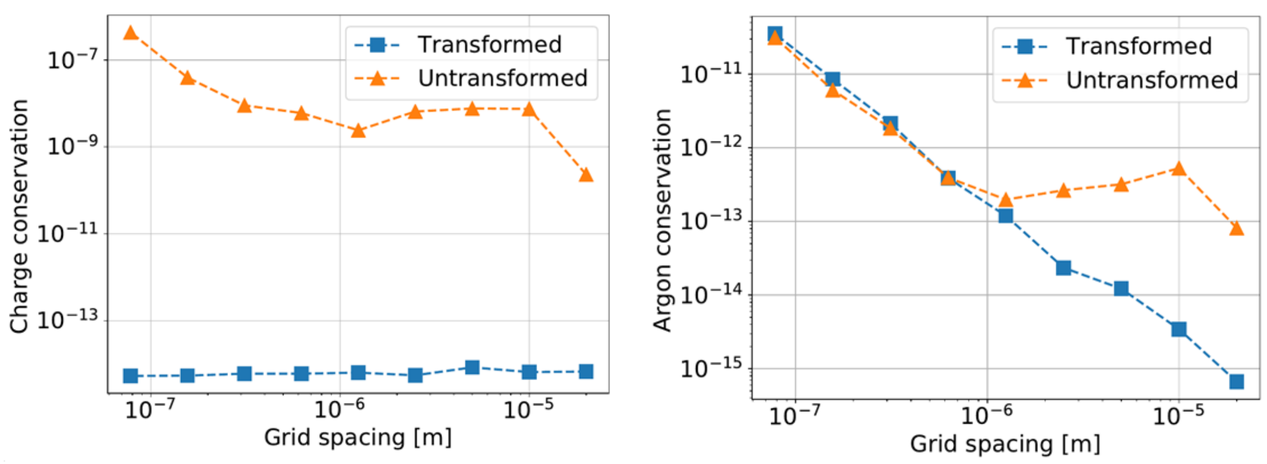
Untransformed Transformed

Untransformed Transformed

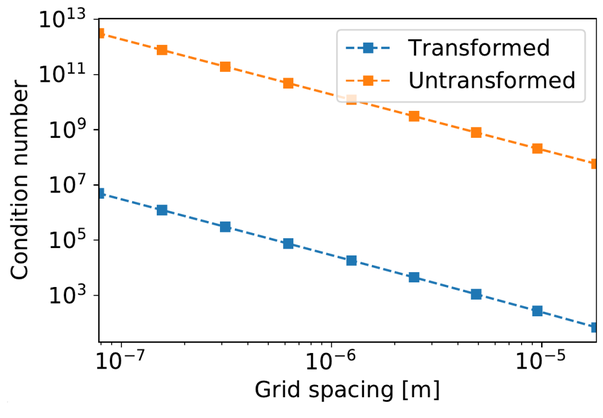


4. Numerical results argon case

Charge & argon conservation improved



Condition number discretization matrix decreased



Smaller condition number:
- Less sensitive to arithmetic errors
- Faster convergence of iterative linear solvers

5. Conclusion & outlook

- Stoichiometry used to transform system

- Transformed system partly source-free

- Numerically favorable properties for example system

- Apply to complex chemistry (CO_2)

- Exploit source-free set in solution procedure

- Transformation not unique, further optimization possible?

Acknowledgements

This research is supported by the Netherlands Organisation for Scientific Research (NWO), which is partly funded by the Ministery of Economic Affairs. The Netherlands eScience Center in the framework of the JCER program. The Netherlands eScience Center is funded by NWO and SURF.

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[3] Krautle, Knabner (2007) A reduction scheme for the coupled multicomponent transport-reaction problems in porous media