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A PLASIMO global model for plasma assisted CO₂ conversion

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Motivation

 Plasma assisted CO₂ conversion is a hot topic in recent plasma research, in which modeling plays an important part, but:

 rich (CO₂) chemistry + modeling = difficult

In general, two options:
1. Simplify type of model: global model
2. Simplify chemistry: reduce species/reactions

Aim of this model:
• PLASIMO global model with complex chemistry set
• Study chemistry and apply advanced mathematical reduction technique ILDM (see poster GT1.00062)

Model based on CO₂ model by Kozák1 (based on Aerts2) implemented in the established code GlobalKIN3, additional aim:
• cross-validate models

Chemistry

Current model 43 species:

CO₂, CO, C, C₂, O, O₃, O₂⁺, C⁺, C₂O⁺, C₂O₂⁺, CO⁺, CO₂⁺, CO³⁺, O⁺, O₂⁺, O₃

interacting in 395 reactions (see background).
Goal is extension with 29 vibrational species (20 CO₂, 9 CO) and appropriate reactions.

Preliminary results

Time response to triangular pulse:

Aerts:

Outlook

• Cross validation with other models; confirming chemistry.
• Apply reduction techniques (ILDM) for application in higher dimensional models.

1 Tomáš Kozák and Annemie Bogaert, Splitting of CO₂ by vibrational excitation in non-equilibrium plasmas: a reaction kinetics model, 2014, Plasma Sources Sci. Technol. 23 045004