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A PLASIMO global model for plasma assisted CO\textsubscript{2} conversion

Wouter Graef, Tafizur Rehman, Diana Mihailova, Jan van Dijk

Motivation

Plasma assisted CO\textsubscript{2} conversion is a hot topic in recent plasma research, in which modeling plays an important part, but:

rich (CO\textsubscript{2}) 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 CO\textsubscript{2} model by Kozák\textsuperscript{1} (based on Aerts\textsuperscript{2}) implemented in the established code GlobalKIN\textsuperscript{3}, additional aim:
• cross-validate models

Chemistry

Current model 43 species:
\[
\begin{align*}
\text{CO}_2, \text{CO}, \text{O}, \text{O}_2, \text{O}_4, \text{O}_5, \text{O}_6, \\
\text{C}_2, \text{C}_2\text{O}_4^+, \text{C}_2\text{O}_4^+, \text{C}_3\text{O}_4^+, \\
\text{CO}_3^+, \text{CO}_3^+, \text{CO}^+, \text{O}_a^+, \text{O}_2^+, \text{O}^- \\
\end{align*}
\]

interacting in 395 reactions (see background).
Goal is extension with 29 vibrational species (20 CO\textsubscript{2}, 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.

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\textsuperscript{1} Tomáš Kozák and Annemie Bogaert, Splitting of CO\textsubscript{2} by vibrational excitation in non-equilibrium plasmas: a reaction kinetics model, 2014, Plasma Sources Sci. Technol. 23 045004

\textsuperscript{2} Aerts R, Martens T and Bogaerts A, Influence of Vibrational States on CO\textsubscript{2} Splitting by Dielectric Barrier Discharges, 2012 J. Phys. Chem. C 116 23257

\textsuperscript{3} ajesh Dorai, Modeling of Atmospheric Pressure Plasma Processing of Gases and Surfaces, Ph.D. Thesis, University of Illinois: Urbana-Champaign, 2002