A PLASIMO global model for plasma assisted CO2 conversion

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Motivation

Plasma assisted CO_2 conversion is a hot topic in recent plasma research, in which modeling plays an important part, but:

rich (CO_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:

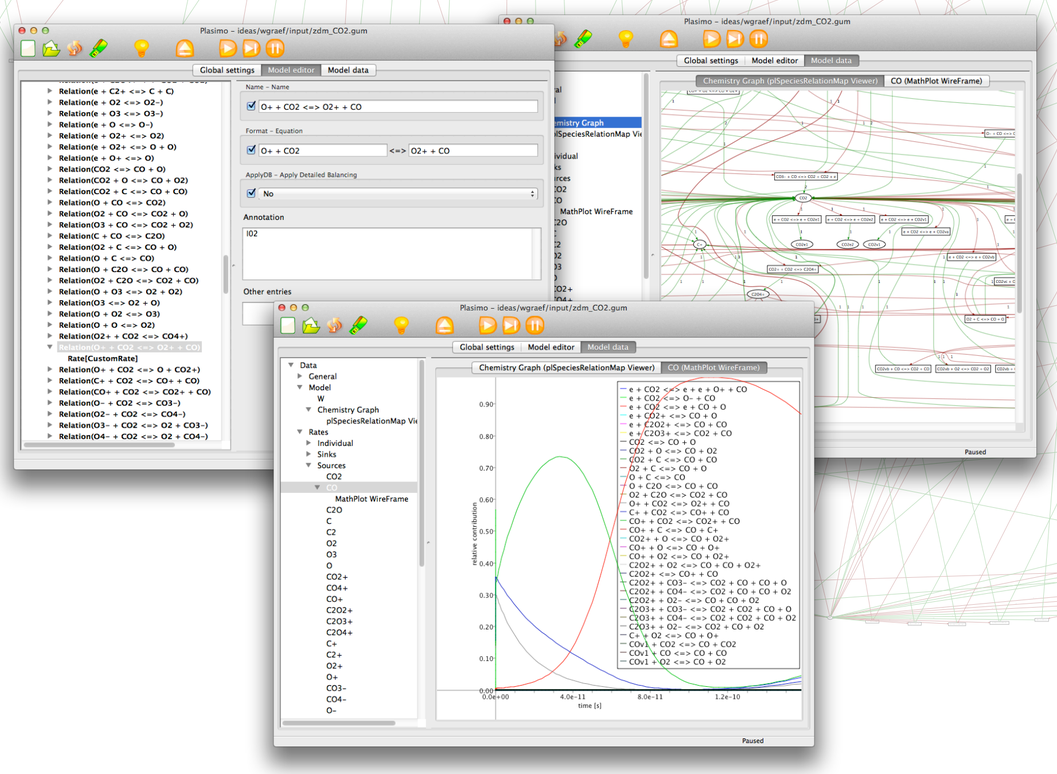
- PLASIMO global model with complex chemistry set
- Study chemistry and apply advanced mathematical reduction technique ILDM (see poster GT1.00062)

Model based on CO_2 model by Kozák[1] (based on Aerts[2]) implemented in the established code GlobalKIN[3], additional aim:

- cross-validate models

PLASIMO global model module

PLASIMO is a highly modular modeling framework for low temperature plasma sources implemented in C++ (see also GT1.00056). The global model module solves balances for species densities and electron energy density (assuming Maxwellian EEDF) as function of time.



PLASIMO graphical user interface

Chemistry

Current model 43 species:

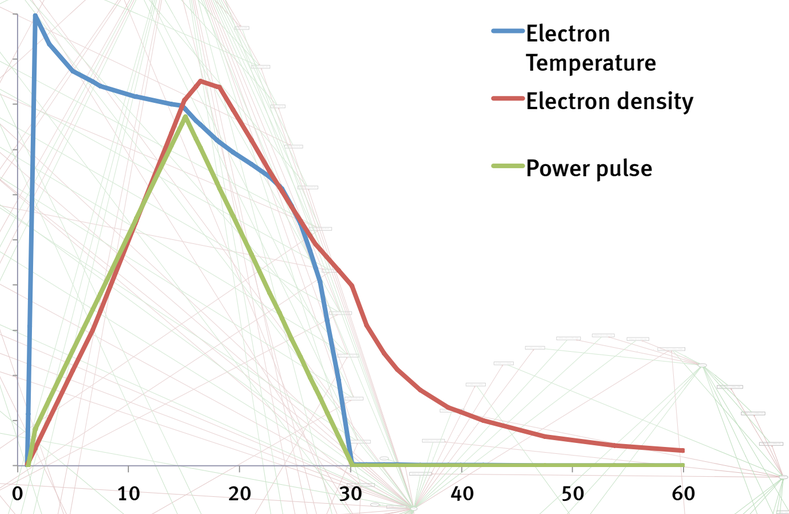
CO_2 (7), CO (6), C_2O, C, C_2, O, O_2, O_3	CO_3^-, CO_4^-, O^-, O_2^-, O_3^-, O_4^-	C_2^+, C^+, $C_2O_4^+$, $C_2O_3^+$, $C_2O_2^+$, CO_4^+, CO_2^+, CO^+, O_4^+, O_2^+, O^+

interacting in 395 reactions (see background).
Goal is extension with 29 vibrational species (20 CO_2, 9 CO) and appropriate reactions.

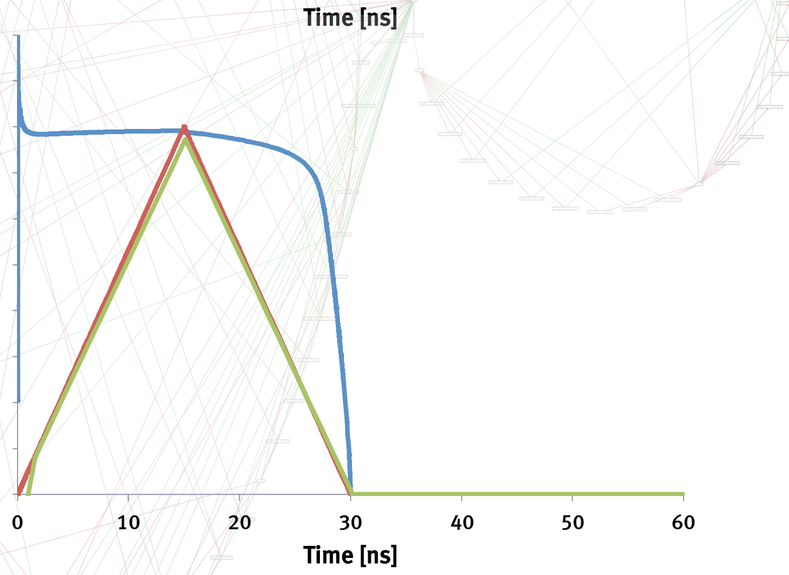
Preliminary results

Time response to triangular pulse:

Aerts:



PLASIMO:



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 CO_2 by vibrational excitation in non-equilibrium plasmas: a reaction kinetics model, 2014, *Plasma Sources Sci. Technol.* **23** 045004

[2] Aerts R, Martens T and Bogaerts A, Influence of Vibrational States on CO_2 Splitting by Dielectric Barrier Discharges, 2012 *J. Phys. Chem. C* **116** 23257

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