

A PLASIMO global model for plasma assisted CO₂ conversion

Citation for published version (APA):

Graef, W. A. A. D., Rehman, T., Mihailova, D. B., & Dijk, van, J. (2014). *A PLASIMO global model for plasma assisted CO₂ conversion*. Sessuin GT1-. Poster session presented at 67th Annual Gaseous Electronics Conference, GEC2014, 2-7 November 2014, Raleigh, North Carolina, United States, Raleigh, North Carolina, United States.

Document status and date:

Published: 01/01/2014

Document Version:

Accepted manuscript including changes made at the peer-review stage

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

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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:

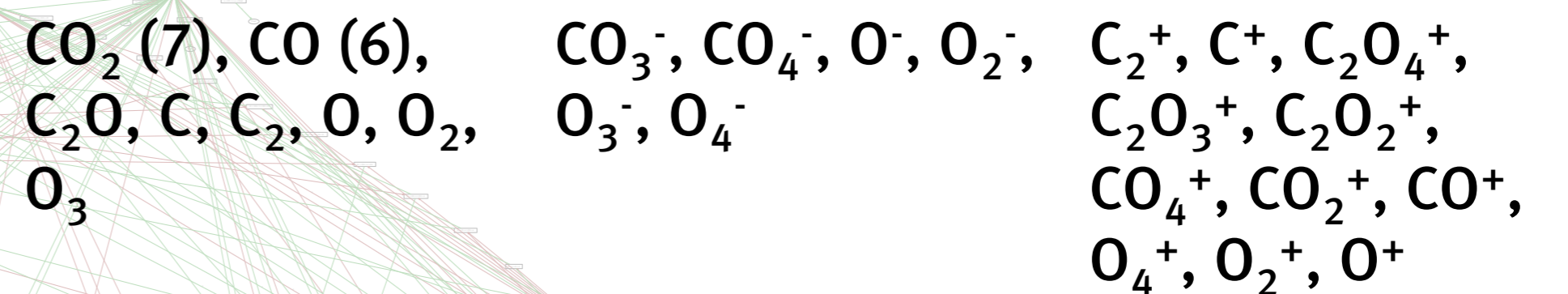
- cross-validate models

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.

Chemistry

Current model 43 species:



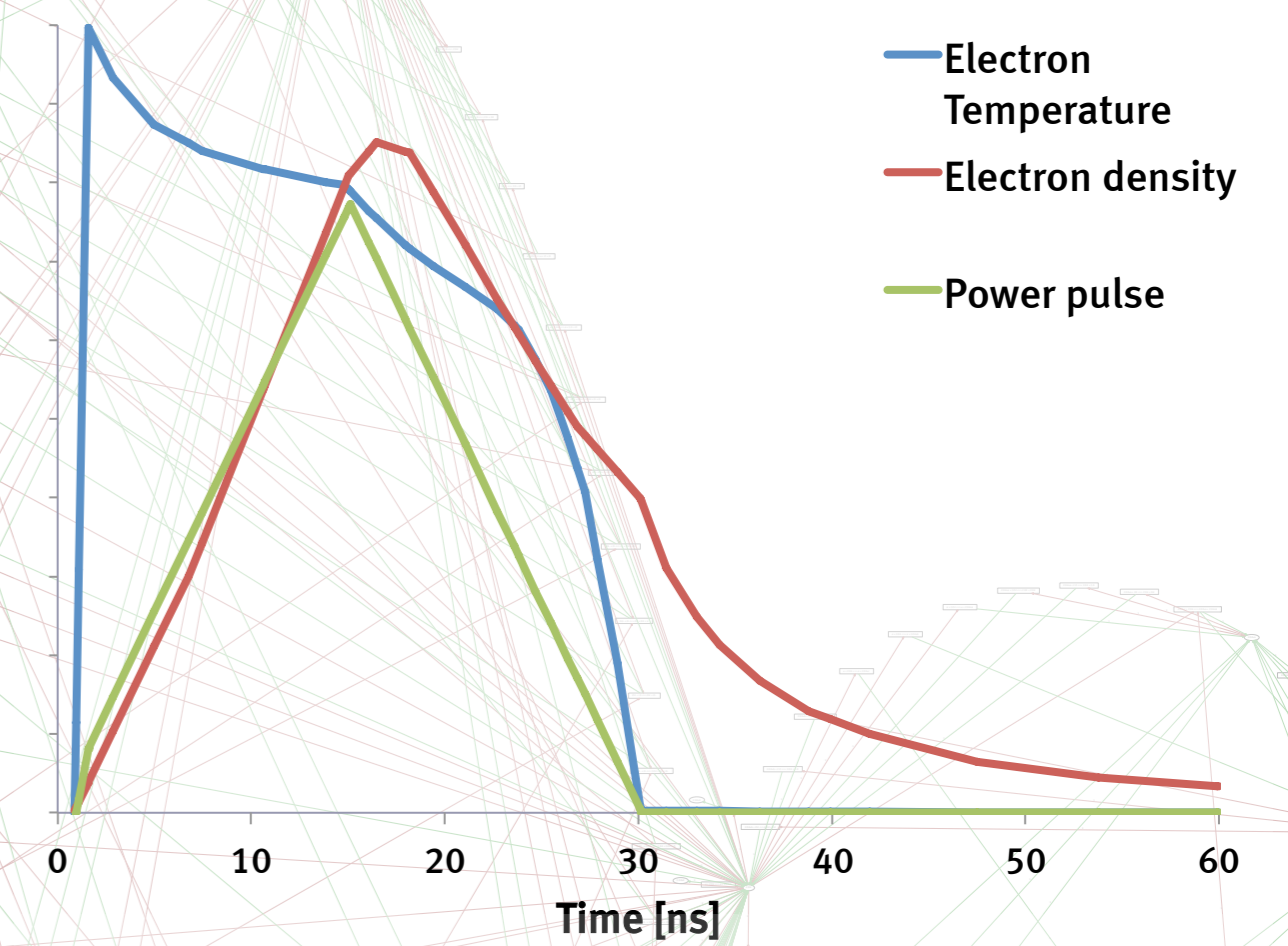
interacting in 395 reactions (see background).

Goal is extension with 29 vibrational species (20 CO₂, 9 CO) and appropriate reactions.

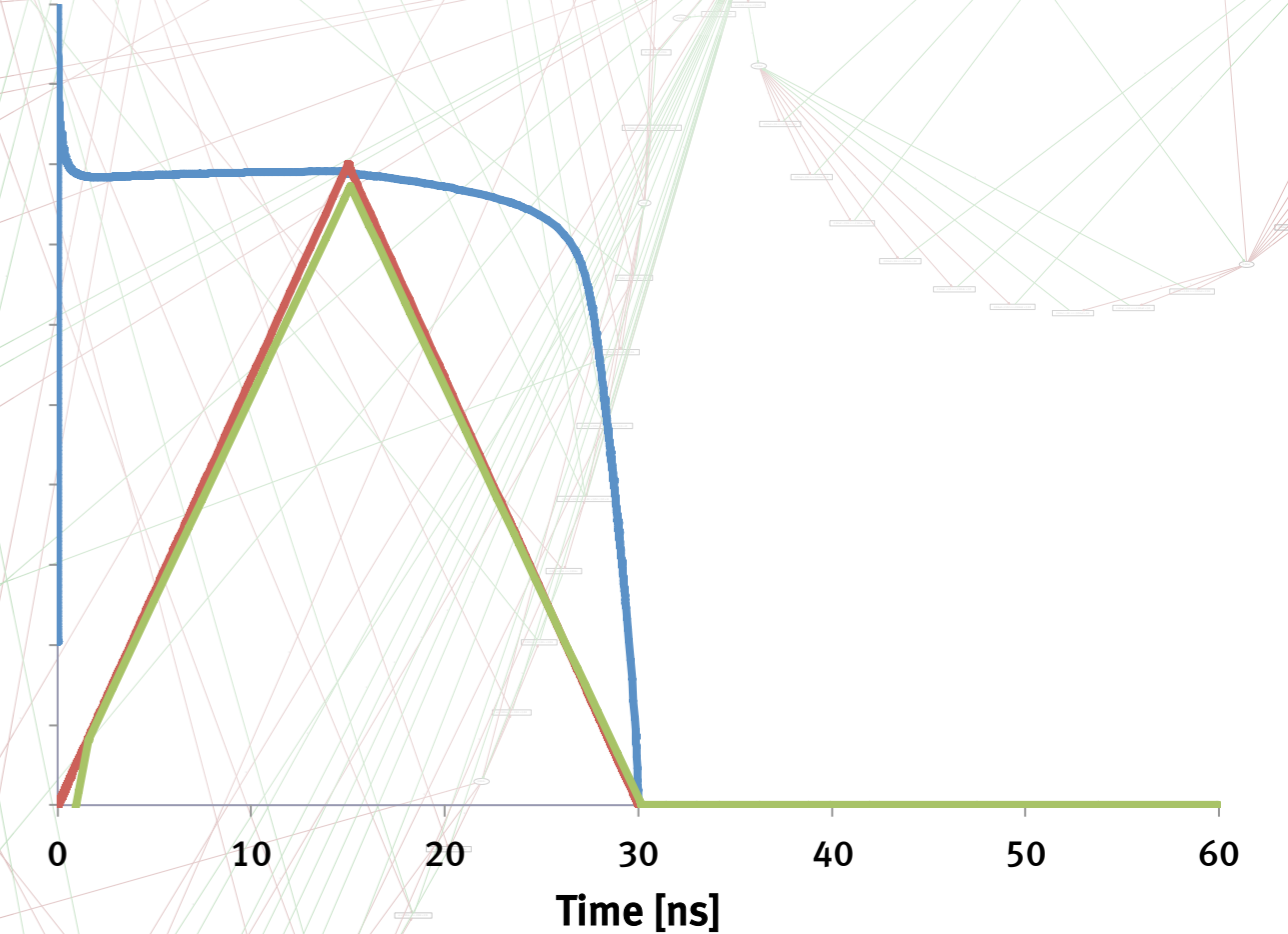
Preliminary results

Time response to triangular pulse:

Aerts:



PLASIMO:



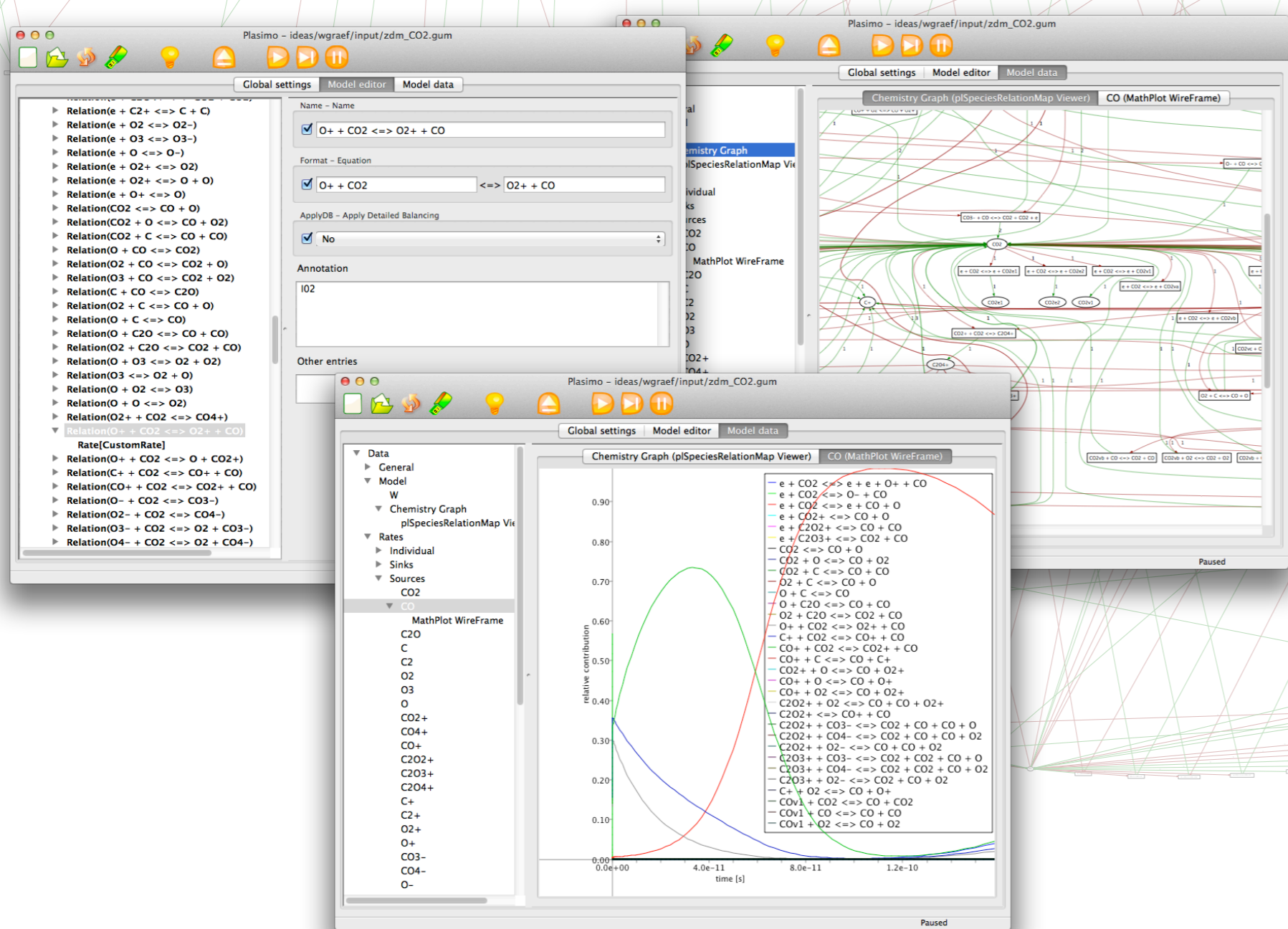
Outlook

- 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 CO₂ 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 CO₂ 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



PLASIMO graphical user interface