Ministry of Human Resources and Social Security

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

2020 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project: Contraction of a microwave heated CO_2-plasma – extending a plasma chemistry model by a two-dimensional discharge contraction model

Helmholtz Centre and institute: Forschungszentrum Jülich GmbH - IEK-4

Project leader: Dr. Dirk Reiser

Web-address: https://www.fz-juelich.de/iek/iek-4/DE/Home/home_node.html

Description of the project:
There is a growing interest in the use of plasma technology for CO_2 conversion inspired by the potential significance of this process for production of synthetic fuels and chemicals (Power-to-X). Non-thermal microwave sustained plasmas offer an attractive scenario to accomplish this task. At IEK-4 numerical tools have been developed which allow the analysis of CO_2 conversion in the gas phase with and without a catalyst. The underlying models are based on reaction kinetics which is a natural starting point to identify fundamental processes in a complex system where many reactions appear simultaneously. On the one hand the predicitive modelling tools cover the simulation of chemical processes for a given set of reaction coefficients. On the other hand model discovery tools will be applied to analyse the data from plasma experiments (concentrations of different gas species and coverage of catalyst surfaces) to obtain the rate coefficients which form the concrete reaction kinetics model. At present many reaction mechanisms and corresponding rate coefficients are not known a priori and have to be extracted from experiments. For this purpose a gas phase code has been coupled with a simplified 1D flow model. However, experimental observations have shown that microwave heated plasmas tend to contract at certain levels of pressure and, therefore, it is needed to take into account a much more complex plasma dynamics in a realistic simulation of the interplay of plasma chemistry and plasma flow. In this project it is planned to implement a detailed and selfconsistent 2D model of a CO_2 plasma column, which includes a mechanism of plasma contraction. The task consists of literature research to compare existing models, implementation of the model in the existing code framework and numerical tests to prove the validity of the model compared to experimental data.

Description of existing or sought Chinese collaboration partner institute:
Our team is looking for a Chinese collaboration partner institute on the research topic described above.

Required qualification of the post-doc:

- PhD in physics, chemistry or enginnering
- Experience with plasma chemistry and computational fluid dynamics
- Additional skills in FORTRAN or a similar programming language

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team