Predictions of NOx-emissions in combustion processes using chemical reactor networks

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Introduction

CFD simulations can only partially support the design of new technologies and plant concepts, i.e. planners must limit themselves to the detailed simulation of plant components or individual reactors. On the other hand, it is necessary to consider the overall plant and system behaviour in order to evaluate different configurations. For this type of overall analysis, commercial 1D software tools such as IPSEpro or Aspen is generally used, which allow a holistic description of the plants with predefined industrial standard reactor types and modules. However, new reactor concepts or designs can only be represented to a limited extent in these calculation tools. Furthermore, these utilities are not able to predict all relevant process variables (fine dust, tar content and NOx emission), so that a complete process evaluation is not possible. Hence, new process models must be developed and existing modules have to be adapted for these purposes.

Project aims

Detailed CFD simulations of single reactor compartments will be used to map the numerical results into specific 0D/1D models. For thermochemical conversions, typically reactor networks of simple reactor types (CSTR, PFR) are planned as a basic model concept.

Therefore, this project aims to develop a suitable (if possible automated) methodology to use detailed CFD model results as well as experimental data to develop simplified 0D/1D models or model networks for specific plant types which are based on physically correct flow structures, heat transfer mechanisms or chemistry-turbulence interactions. These modules are then planned to be interconnected within the framework of a modular development environment. The methodology for generating a chemical reactor network (CRN) is shown in Fig. 1.

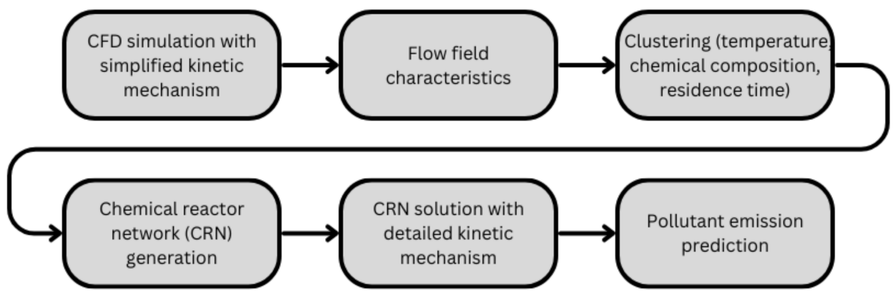

Fig. 1: Principle scheme of transferring CFD results into reactor-networks.

In order to guarantee a high degree of user-friendliness, commercial tools such as IPSEpro are planned to be used as user interface.

Methodology

The clustering of CFD data and assembly into a CRN is performed using NetGEN, a software package designed for the automated generation of CRNs. [1] A schematic representation of a CRN in the secondary combustion chamber of a biomass furnace is shown in Fig. 2.

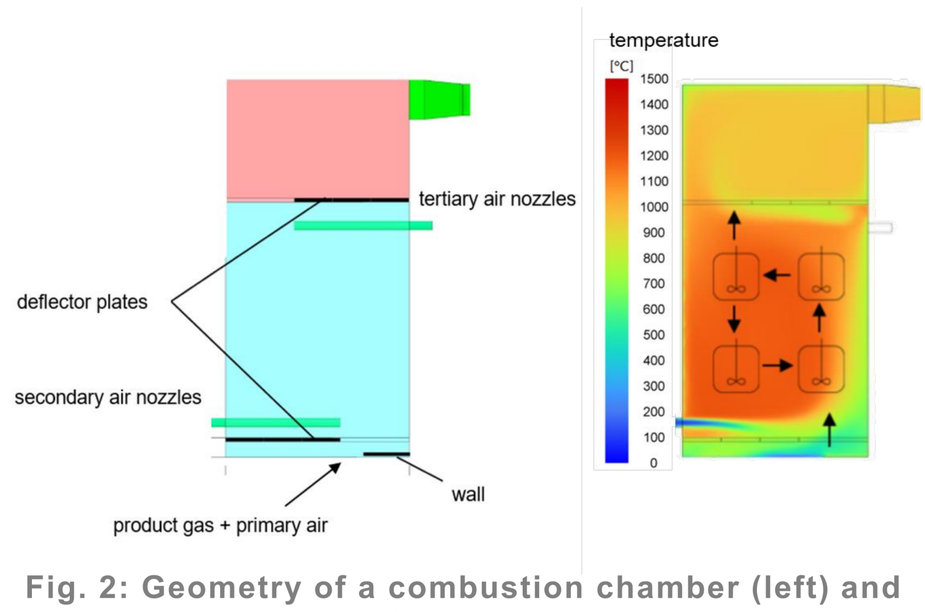

Fig. 2: Geometry of a combustion chamber (left) and representation of a CRN based on the temperature field (right)

Preliminary results

The cluster method is being tested and validated for two industrial applications (biomass furnace, cement burners).

Biomass furnace (5 reactors)

The mass flows between the clusters are evaluated. Each cluster (Fig. 3) represents a single reactor within the reactor network.

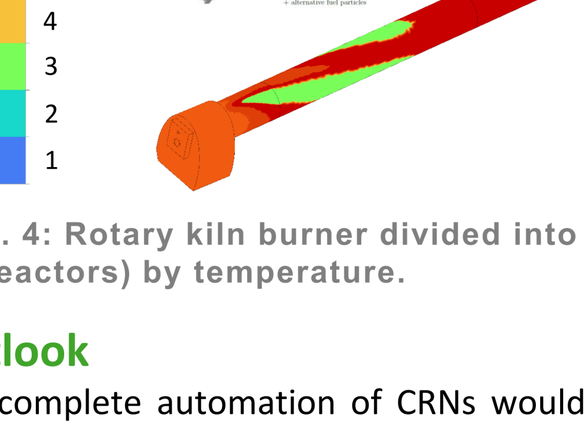

Fig. 3: Biomass furnace divided into 5 clusters (=reactors) by temperature and main nitrogen-species.

Rotary kiln burner (7 reactors)

Due to the high temperatures present within the rotary kiln burner, the predominant pollutant generated is thermal NOx, which is largely dependent on the temperature (Fig. 4)

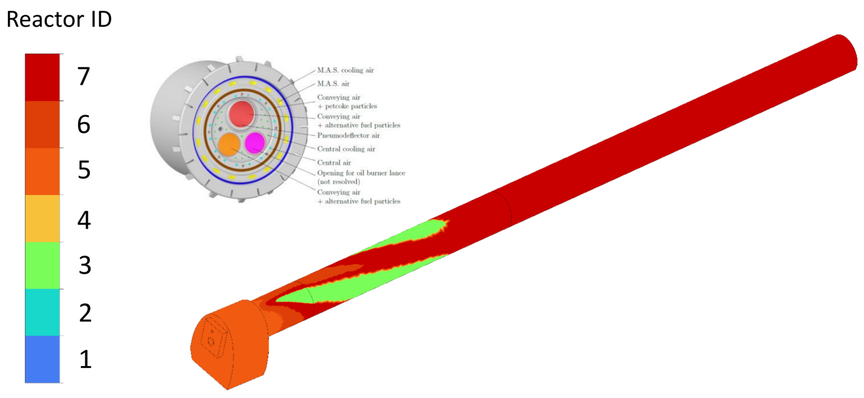

Fig. 4: Rotary kiln burner divided into 7 clusters (=reactors) by temperature.

Outlook

The complete automation of CRNs would be beneficial in accelerating the prediction of NOx emissions, thereby conserving computational resources.

References:

[1] M. Savarese, A. Cuoci, W. De Paepe, A. Parente (2023) Machine Learning clustering algorithms for the automatic generation of chemical reactor networks from CFD simulations Fuel, 343

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