Influence of CFD-CRN clustering parameters on the prediction of NO_X emissions

Author:
Michael Eßl
Magdalena Krainz
Thomas Steiner

SUBAREA 2.1: Process Analysis and Simulation

Introduction

Computational Fluid Dynamics (CFD) represents the state of the art for optimization and design of biomass furnaces. The major species of the combustion process such as CO, CO_2, H_2, CH_4, H_2O, O_2 and N_2 can be adequately described by simple global reaction mechanisms. In contrast, NO_X emissions, especially from fuel-bound Nitrogen, cannot be accurately predicted by simple mechanisms. For the accurate prediction of NO_X emissions over a wide range of operating conditions detailed reaction mechanisms with more than 100 species and 1000 reactions are necessary. These mechanisms are too computationally expensive for direct implementation in CFD. Therefore, the chemical reactor networks (CRN) method is applied which solves the complex reaction mechanism using a network of idealized continuously stirred tank reactors (CSTR). The generation of the network is the major challenge in the CRN method. The present study utilizes datasets extracted from simple combustion CFD simulations and the process for this CFD-CRN coupling is shown in Fig. 1. The focus of the study is on the clustering step that defines the volumes, temperatures, and connection of the reactors.

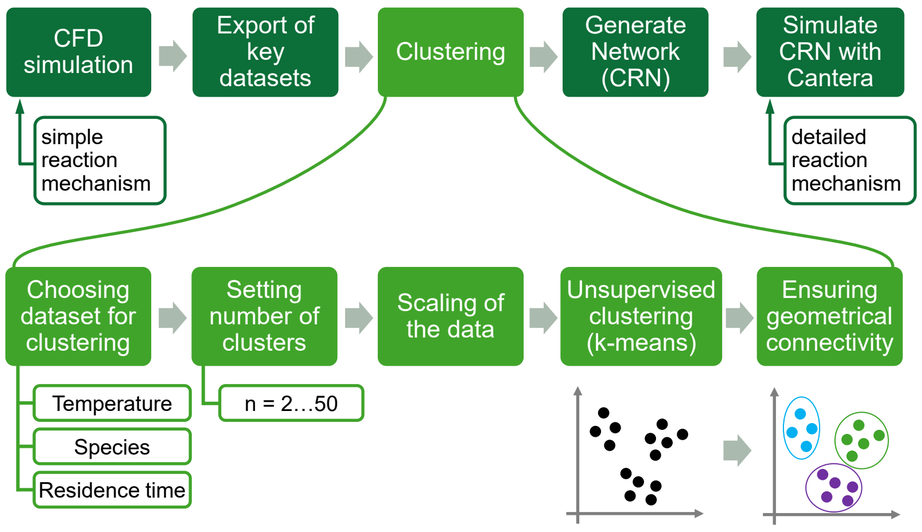


Fig. 1: Procedure for reactor network generation [1]

Methodology

As a case study, the secondary combustion zone of a pellet furnace was investigated (Fig. 2) and the CFD-CRN coupling was performed in three-steps.

Step 1: CFD simulation of combustion in the furnace with simple reaction mechanism.

Step 2: Extraction of datasets (temperature, residence time, O_2 concentration, position) from CFD results and clustering using the k-means algorithm with predefined settings (i.e., number of reactors) implemented in NetGEN [2]. Each reactor is defined by a fixed volume, temperature and, its connections to inlets, outlets and neighboring reactors.

Step 3: Solution of the reactor network using detailed reaction mechanisms in the Cantera software package.

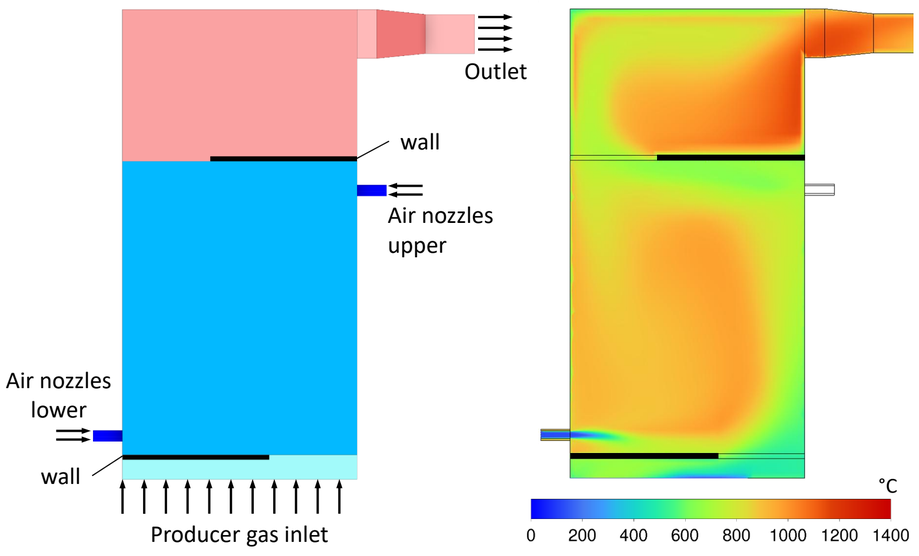


Fig. 2: CFD - simulation domain (left) and resulting temperature field of combustion simulation (right) [2]

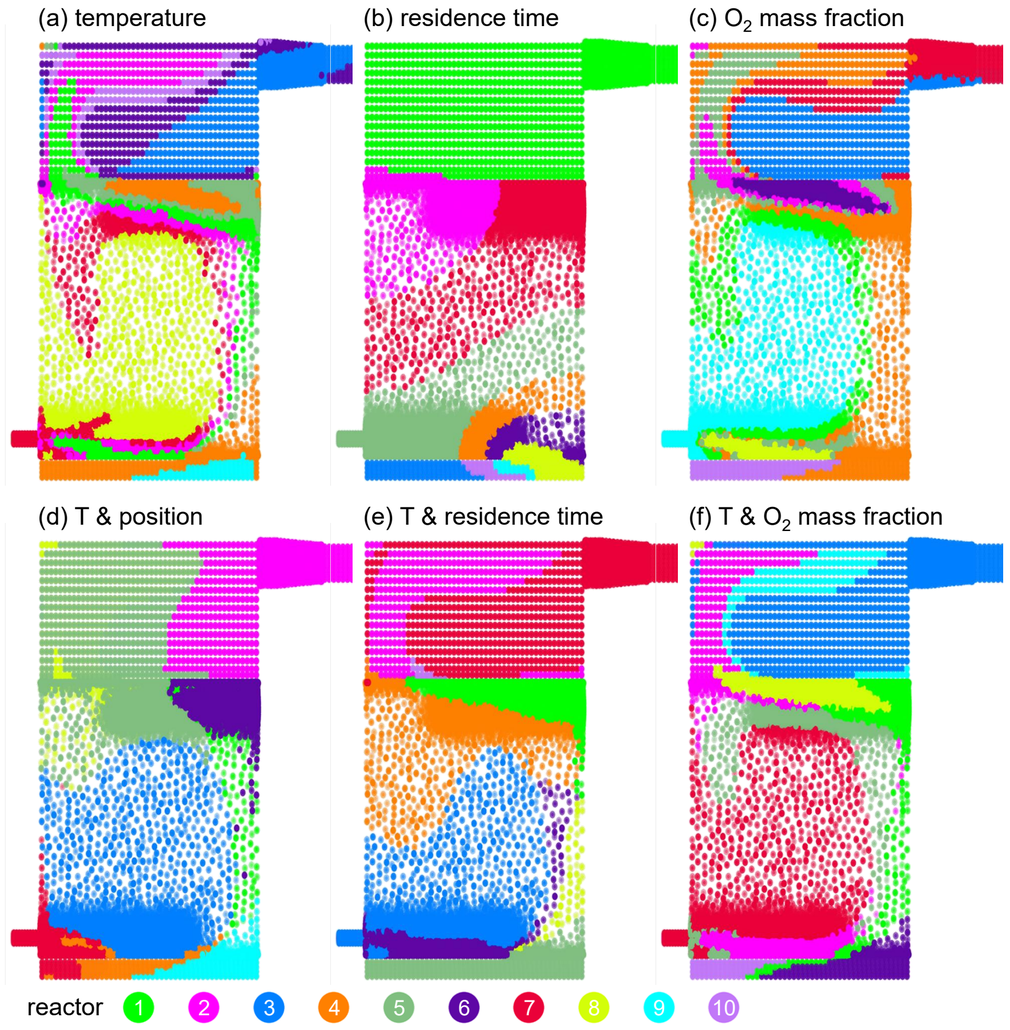


Fig.3: Clustering results for 10 reactors with single (a-c) and combined (d-f) CFD datasets; T... temperature

Results

The CFD datasets selected for clustering significantly influence the resulting reactor network (Fig. 3) and, consequently, the predicted NO_X emissions (Fig. 4). The networks based on temperature (a) and O_2 (c) show similar structures, indicating a strong relationship between these datasets i.e., high temperatures occur in oxygen-depleted zones. In contrast, the residence time resulted in reactors distributed along the flow path in the furnace, yielding a cascade-like arrangement of CSTRs. The best agreement of predicted NO_X emissions with the CFD results was obtained using residence time and the combination of temperature and position datasets.

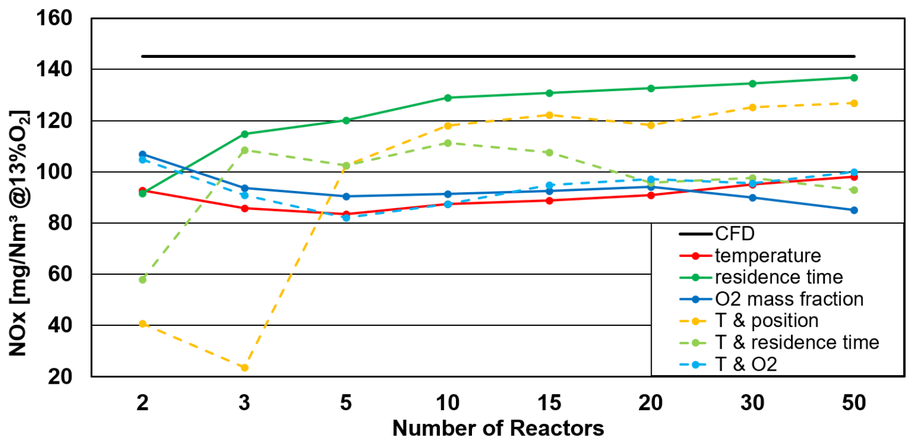


Fig.4: Influence of the reactor network size and CFD datasets used in clustering; T... temperature

Outlook

In addition to the selected CFD datasets, the influence of the clustering algorithm should be investigated. The focus should be on algorithms capable of determining the required number of reactors for given geometries and operating conditions thereby reducing the number of user-defined clustering parameters.

References:

[1] Krainz, M. (2025). Predictions of NO_X-emissions in combustion processes using chemical reactor networks [Master thesis, Graz University of Technology]

[2] Savarese, M., Cuoci, A., De Paepe, W., Parente, A., (2023) Machine Learning clustering algorithms for the automatic generation of chemical reactor networks from CFD simulations. Fuel, 343, Article 127945. https://doi.org/10.1016/j.fuel.2023.127945

BEST – Bioenergy and Sustainable Technologies GmbH

Head Office Graz
Inffeldgasse 21b
A 8010 Graz

P +43 5 02378-9201
office@best-research.eu
www.best-research.eu

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