Numerical investigation of reaction mechanisms on NO_x emissions from biomass combustion with enhanced reduction

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AREA 2.1 Process Analysis and Simulation

Introduction

With the increasing demand for lower emissions and innovative combustion technologies, it is necessary to have a reaction mechanisms that is accurate as well as computationally affordable for geometry and process optimization using computational fluid dynamics (CFD). The objective of this work is to explore the applicability of several reaction mechanisms in predicting NOx emissions from various combustion systems. This work focuses on the selection of suitable mechanisms from literature (see Table 1) in a full scale 3D model for the prediction of NO_X especially for furnaces with low oxygen concentration in the fuel bed and enhanced reduction zones.

Table 1: Data of the investigated reduced and detailed reaction mechanisms

Name	No. species (total / N species)	No. reactions	Note	Release year
Gbg	148 / 82	2764	up-to-date detailed mechanism	2018
GRI	48 / 16	634	older detailed mechanism	1999
Li	35 / 14	304	derived from Gbg	2019

Explanation: The *total* number of species exclude inert species (Argon (Ar), Helium (He), and N_2). The number of nitrogen containing species (*N species*), also exclude N_2. The number of reactions counts reversible reactions as two separate reactions.

Methodology

We conducted numerical investigations using chemical reaction kinetic simulations with continuous stirred tank reactor networks (see Figure 1). The network consists of two reactors representing the Secondary Combustion Zone (SCZ) and Tertiary Combustion Zone (TCZ). The composition of the producer gas is taken from measurements. Since the measurement data contain tars, a simple tar cracking model is applied to get a suitable producer gas composition for the simulations. The modified producer gas is than diluted with air to get the desired air-to-fuel equivalence ratio (λ) and fed into the reactor representing the SCZ.

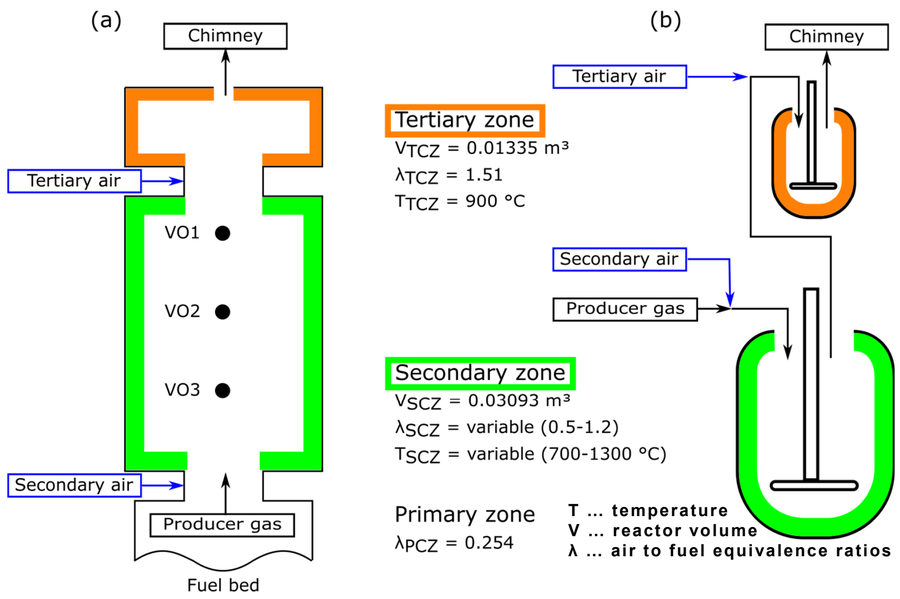

Figure 1: (a) Scheme of the experimental prototype; (b) Reactor network used to model the furnace

Results and discussion

First, we compared the predictions of NO_X emissions from a detailed benchmark mechanism (Gbg) with experimental data, analyzing temperature and air-to-fuel equivalence ratio (see Figure 2). The general trend of the emissions is predicted well considering the simplifications and assumptions of ideal reactors.

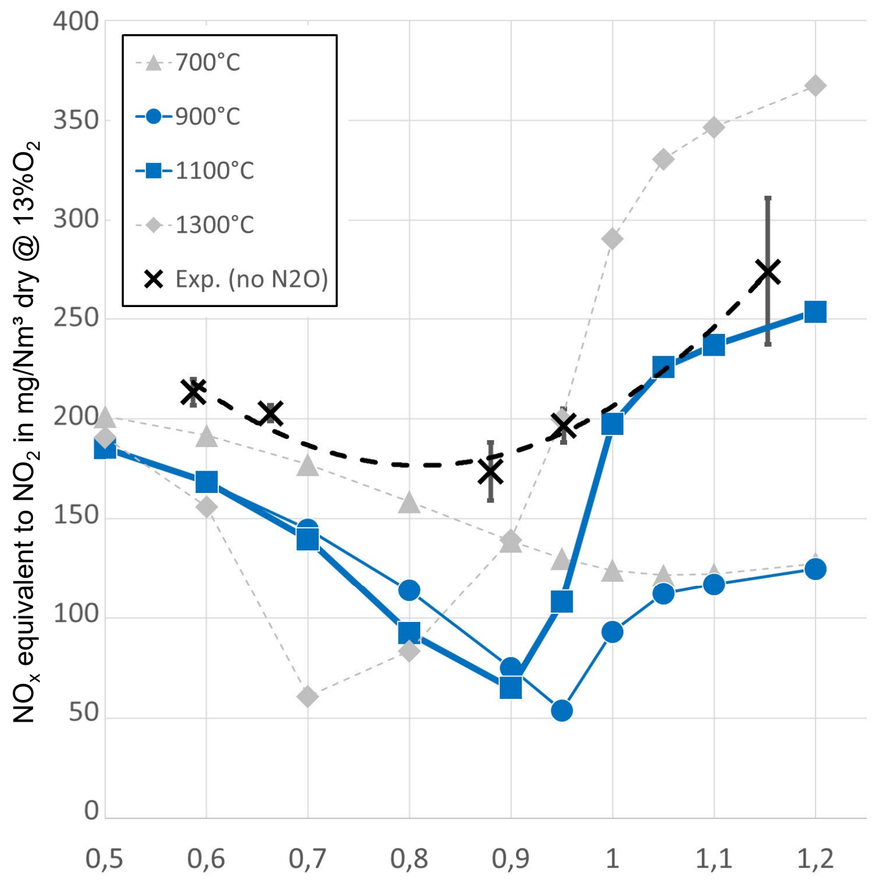

Figure 2: NO_X emissions from measurement and reaction kinetic simulation; measured temperature range 900-1100°C;

Subsequently, we compared two mechanisms, GRI and Li, that are applicable in CFD with the benchmark (Gbg) mechanism (see Figure 3). At high λ and high temperature conditions all mechanisms predict a similar trend of the NO_X and precursor species. At low λ and low temperature conditions there are deviations from the benchmark that are higher for the GRI than the Li mechanism. Therefore, only the Li mechanism is able to predict NO_X and their precursors accurately enough. Currently the Li mechanism is validated in CFD simulations for various low NO_X combustion concepts.

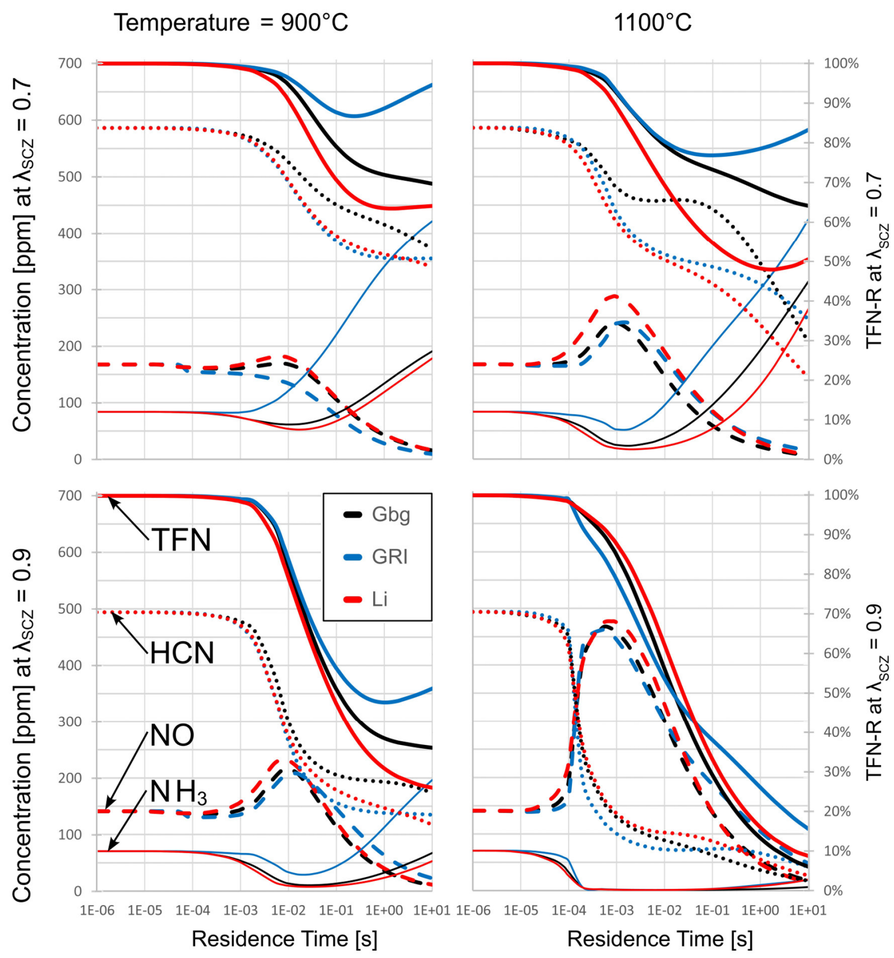

Figure 3: Comparison of several reaction mechanisms in terms of NO, NH_3, HCN and TFN over residence time; ppm on dry basis;

Further details and references are shown in the submitted publication that is currently under review.

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