

# Comparison of reduced mechanisms for gasifying applications

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**Abstract**—A detailed 26-step heterogeneous mechanism for char gasification is reduced. Reduction is carried out based on sensitivity and reaction flow analysis. The reduced mechanism is then used in three different numerical tools of varying detail to analyze its performance and sensitivity to boundary conditions and treatment of external influences.

## I. INTRODUCTION

Present detailed mechanisms for biomass and coal conversion in combustion and gasification applications are too time-consuming for large scale CFD simulations with a high number of particles. Our goal is to develop a reduced heterogeneous mechanism for solid fuel conversion in combustion or gasification environments with sufficient accuracy and low computational cost applicable in engineering tools. Starting point for the reduction is the 26-step char conversion mechanism developed at Stanford University [1] which was obtained using Thermogravimetric Analysis (TGA) of Wyodak coal. For gas phase reactions, GRI 3.0 [2] is used. We reduce the mechanism via sensitivity and reaction flow analysis using the commercial software LOGEsoft [3] and compare with TGA results of the Sandia group, data from the stand-alone code for particle conversion called Stanford-code [4] and the implementation of the Stanford-code into the open source CFD software Pencil-code developed at NTNU.

The mechanism assumes that the coal has already undergone the processes of devolatilization and pyrolysis, so that only pure char is present. This char comes in two distinct phases; one represents carbon atoms that have contact to the gas phase, on the surface and in the pores of the char particle, and the other represents the bulk phase beneath it. As surface carbon atoms desorb into the gas phase, the underlying bulk phase atoms become the surface phase.

## II. METHOD

### A. Reduction

The chemical analysis suite LOGEsoft provides sensitivity and reaction flow analysis for heterogeneous and homogeneous mechanisms. Given the Arrhenius expression for a reaction rate  $k$

$$k = Ae^{-\frac{E_a}{RT}} \quad (1)$$

with  $A$  being the preexponential factor,  $E_a$  the activation energy,  $R$  the gas constant and  $T$  the absolute temperature, sensitivity analysis provides data on how a change in the reaction rate affects a target attribute of the flow, e.g. outflow temperature or water vapor fraction. Reaction flow analysis looks at which rate a reaction occurs under the boundary conditions applied. The importance of a reaction for the overall mechanism is assessed using these two methods and a reaction is neglected if it is deemed not important.

### B. Simulations

The reduced mechanisms obtained are supplied to three numerical tools with varying degree of detail for fluid-solid interaction: the LOGEsoft gasifier module, the Stanford-code and the open-source CFD code called Pencil-code.

1) *Gasifier module of LOGEsoft*: The module treats the gasifier as a series of Partially Stirred Reactors (PaSR), where turbulence effects are taken into account through a stochastic mixing model [5]. The gas in each PaSR is divided in a number of virtual gas particles which in turn contain solid particles. Radiation and mixing are described by probability density functions, so that two gas particles mix attributes of the gas phase or exchange heat with the gasifier wall randomly. The solid matter particles are modeled as moving with the surrounding gas and their total surface sites are governed by their weight, specific surface and porosity. The gasifier and particles are not resolved spatially.

2) *Stanford-code*: A thorough description of the code can be found in [6]. The code assumes a cloud of particles of uniform size and behavior in quiescent gas. It takes particle-particle, particle-fluid and particle-wall radiation into account and treats the particles as 0-dimensional. The influence of internal gradients on particle conversion are modeled by applying a Thiele modulus [7]. The near-field gas composition around the particle is calculated using an equilibrium assumption. Stokes flow is taken into account, reversible reaction rates are calculated using an equilibrium constant calculated from the change in Gibbs free enthalpy over the reaction. With the current heterogeneous mechanism it is able to predict mass loss rates of Wyodak char well.

3) *Pencil-code*: The Pencil-code is a open-source CFD code capable of large-scale Direct numerical simulation (DNS) [8]. It uses lagrangian tracking of the particle phase

TABLE I  
BOUNDARY CONDITIONS FOR SIMULATIONS

Condition	Value
$T_{gas}$	1640K
$T_{part}$	1640K
$r_{part}$	$50\mu m$
$Y_{H_2O}$	0.4
$Y_{O_2}$	0.55
$Y_{N_2}$	0.05

and can simulate up to one million particles. Particle-fluid momentum transfer is calculated using the Stokes drag as the particles in question are very small, of the order  $50\mu m$ . Radiative heat transfer is not yet implemented. The particle chemistry module is based on the Stanford-code and its calculations are carried out for each particle, so a simulation with many particles combined with the detailed mechanism is very costly. A zero-dimensional calculation of the Pencil-code gives the same results as a calculation using the Stanford-code.

### III. SIMULATIONS

To show the promise of the method, we performed three simulations in the Stanford-code with the same boundary conditions: one with the full 26-step mechanism and two reduced, to 7 and 18 steps respectively with a 'best-guess' method. This step will be replaced in the actual contribution by sensitivity and reaction flow analysis. The homogeneous reactions were left unaltered. An overview over the most important conditions can be found in table I.

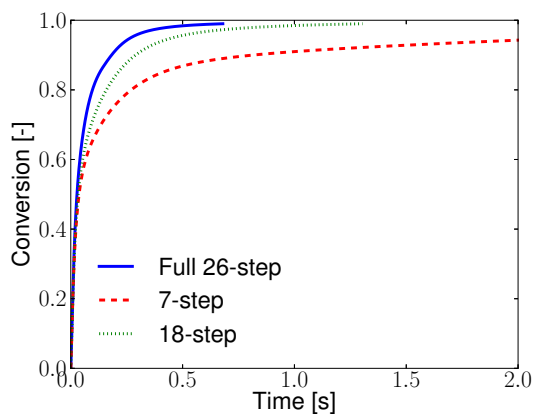


Fig. 1. Particle conversion over time

Figure 1 shows the particle conversion over time for the three cases. All cases agree well until 50% conversion, after that both reduced cases flatten out significantly, with the 18-step mechanism staying closer to the full mechanism. The plots end when 99% conversion has been reached, which was 0.68, 1.3 and 4.7 seconds for the full, 18- and 7-step mechanism.

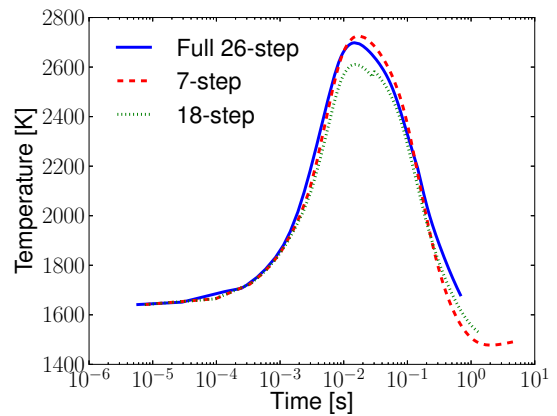


Fig. 2. Particle temperature over time

Shown in figure 2 is the particle temperature evolution over time. The particle temperature of the 7-step mechanism follows the full mechanism closely but has a higher and later maximum, only to fall off faster than the full mechanism. The 18-step mechanism has a significantly lower maximum but follows the full mechanism after 0.1 seconds.

The computational time was 2291 seconds for the 26-step, 573 for the 18-step and 112 seconds for the 7-step without altering GRI 3.0 with its 325 mechanisms. This huge speed up shows the potential that lies in the reduced mechanisms which will be further explored investigating the influence of different sensitivity targets on the predictability of the reduced mechanisms.

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