Progress in Applied CFD – CFD2017
PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focus on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

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**NUMERICAL STUDY OF COAL PARTICLE GASIFICATION UP TO REYNOLDS NUMBERS OF 1000**

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**ABSTRACT**

The influence of turbulent structures on the gasification of coal particles, in particular on the char consumption and surface temperature, is studied. Existing submodels for char gasification are mainly based on results for laminar flow only, therefore the capability of these models to predict gasification at higher particle Reynolds numbers is evaluated using the simulation results. Two representative scenarios were studied: the gasification of a 2 mm particle at atmospheric pressure in a O₂/CO₂/H₂O atmosphere at 2006 K and the gasification of a 263 µm particle at 30 bar in a different O₂/CO₂/H₂O atmosphere at 1480 K. The simulation conditions were based on data obtained from the simulations of two different entrained-flow gasifiers. ANSYS Fluent™ was used to solve the Navier-Stokes equations for the flow field coupled with energy and species conservation equations. The model for the reaction system incorporates six gaseous chemical species H₂, O₂, CO, CO₂, H₂O, N₂ and solid carbon. A semi-global reaction mechanism was applied for the homogeneous gas-phase reactions and the water gas reaction, the Boudouard reaction and the oxidation of carbon to carbon monoxide were considered as heterogeneous gas-solid reactions. In the present work it shows how the reaction zone is modified due to the change in wake structure, the impact of the turbulent effects on the overall carbon conversion rate are discussed, and hints how to adjust existing submodels to correctly predict char conversion at high particle Reynolds numbers are given.

**Keywords:** CFD, gasification, turbulence, heterogeneous reactions.

**NOMENCLATURE**

**Greek Symbols**

- \( \lambda_{ij} \): stochiometric coefficient of species \( i \) in reaction \( j \), [\(-\)]
- \( \theta \): empirical factor, [\(-\)]
- \( \nu \): kinematic viscosity, [\( m^2/s \)]

**Latin Symbols**

- \( c_i \): molar concentration of species \( i \), [\( kmol/m^3 \)]
- \( d_p \): particle diameter, [\( m \)]
- \( k \): reaction rate constant, in SI units.
- \( k_{oo} \): pre-exponential factor, in SI units.
- \( n \): exponent of power law kinetic rate equations, [\(-\)]
- \( p_i \): partial pressure of species \( i \), [\( Pa \)]
- \( p_{op} \): operating pressure, [\( Pa \)]
- \( r \): molar reaction rate, [\( kmol/m^3 \)]

\( u \): magnitude of velocity, [\( m/s \)].

\( D_{eff} \): effective diffusion coefficient in a porous medium, [\( m^2/s \)].

\( E_a \): activation energy, [\( J/kmol \)].

\( K \): inhibition constant, [\( 1/\text{Pa} \)].

\( R \): universal gas constant, [\( J/\text{kmol} \cdot K \)].

\( Re \): particle Reynolds number: \( Re = u_{in} \cdot d_p / \nu \), [\(-\)].

\( S_Y \): Specific surface area per volume, [\( m^2/m^3 \)].

\( X \): char conversion, [\(-\)].

\( Y \): mass fraction, [\(-\)].

**Sub/superscripts**

- \( in \): at the inlet boundary

**INTRODUCTION**

Due to the multiscale character of coal combustion and gasification processes, the use of sub-models describing particle-gas interaction is unavoidable, and the correct prediction of the burning rate and the particle temperature based on this sub-models is an essential part of successfully modeling of such reactors (Edge et al., 2011; Schulze et al., 2013; Richter et al., 2016). An analysis of existing computational burnout sub-models reveals that e.g. the influence of particle velocity on carbon consumption and particle temperature is not well understood. Thus, particle-resolved numerical simulations of single burning particles can highlight different physical phenomena and correlations and therefore they can help to better understand the complex combustion physics. Examples for this approach are given in Refs. (Lee et al., 1996; Higuera, 2008; Kestel et al., 2012; Richter et al., 2013, 2015; Wittig et al., 2016).

To the authors best knowledge almost all single-particle studies published in literature considered laminar flow regimes only and most consider only one heterogeneous reaction i.e. Boudouard, watergas or carbon oxidation. In different technological applications much larger particle Reynolds numbers are possible and all three above mentioned reactions proceed in parallel. For that reason the char-particle burnout corresponding to turbulent flow up to particle Reynolds number equals 1000 in two different O₂/CO₂/H₂O atmospheres is investigated. At these Reynolds numbers time periodicity and the planar symmetry of the vortex shedding are lost and the wake becomes turbulent (Jones and Clarke, 2008; Campregher et al., 2009). The operating conditions, that means pressure, temperature and gas phase composition, are based...
on data obtained from simulations of two different entrained-flow gasifiers.

**MODEL DESCRIPTION**

The gasification is studied for a single spherical particle in embedded in a large domain as schematically shown in Figure 1. As the heterogeneous reaction time scales are much larger than the flow time scales (Sundaresan and Amundson, 1980; Richter et al., 2013), the pseudo-steady state approach was assumed valid, hence no particle-shrinking was taken into account and the steady-state form of the governing equations are solved. Indeed this assumption is confirmed from the simulations results. The lowest value of the ratio of carbon consumption time scale and fluid time scale is found to be of the order $O(10)$, but in most of the cases it is higher. Fluid flow is modelled coupled with species and energy transport as well as coupled with heat conduction inside the solid particle. Buoyancy effects are neglected, hence gravity is set to zero but the density still varies due to e.g. changes in temperature. Turbulence is taken into account using the $k$-$\omega$-SST model in the steady RANS simulations for particle Reynolds numbers larger than $Re = 200$. The Maxwell-Stefan equations are used to describe diffusional mass flux in the multi-component gas mixture and gas-gas radiation is included via the P1 radiation model. The heterogeneous reactions are assumed to take place on the outer particle surface only, however the internal structure of the char particle is considered through an effectiveness factor, which is defined in the next section. The gas phase is modelled as an incompressible ideal gas and all physical properties of the components are modelled using polynomial expressions or kinetic theory. The chemical system incorporates pure carbon as solid and $H_2$, $O_2$, $H_2O$, $CO$, and $CO_2$ as gaseous species. Details of the finite-rate chemical mechanism are discussed in the next section. The process and inlet condition for the two different cases studied in this work are shown in Table 1. Uniform profiles are prescribed for velocity, temperature and species concentrations at the inlet.

### Chemical reactions

The semi-global mechanism to describe the homogeneous gas phase reactions are modelled using a mechanism proposed by Jones and Lindstedt (1988):

\[
\begin{align*}
H_2 + 0.5 O_2 & \rightarrow H_2O, \\
CO + H_2O & \rightarrow CO_2 + H_2.
\end{align*}
\]

Table 1: Process and inlet conditions for both cases considered.

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$dp/m$</td>
<td>$2 \cdot 10^{-3}$</td>
<td>$0.263 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>$P_{op}$/bar</td>
<td>1.013</td>
<td>30</td>
</tr>
<tr>
<td>$T_{in}/K$</td>
<td>2006</td>
<td>1480</td>
</tr>
<tr>
<td>$Re_{in}$</td>
<td>1 – 500</td>
<td>1 – 1000</td>
</tr>
<tr>
<td>$u_{in}/m/s$</td>
<td>0.1932 – 95.58</td>
<td>0.03192 – 31.92</td>
</tr>
<tr>
<td>$Y_{CO, in}$</td>
<td>0.223</td>
<td>0.223</td>
</tr>
<tr>
<td>$Y_{H2O, in}$</td>
<td>0.123</td>
<td>0.221</td>
</tr>
<tr>
<td>$Y_{O_2, in}$</td>
<td>0.366</td>
<td>0.187</td>
</tr>
</tbody>
</table>

Table 2: Kinetic constants for the gas phase reactions.

<table>
<thead>
<tr>
<th></th>
<th>$k_a$, $E_a/(J/kmol)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R1$</td>
<td>5.69 $\cdot 10^{11}$</td>
</tr>
<tr>
<td>$R2$</td>
<td>2.75 $\cdot 10^9$</td>
</tr>
</tbody>
</table>

The Boudouard and water-gas reaction as well as the oxidation of the carbon are considered as heterogeneous reactions of the particles with the gas phase:

\[
\begin{align*}
C + CO_2 & \rightarrow 2 CO, \\
C + H_2O & \rightarrow H_2 + CO, \\
2 C + O_2 & \rightarrow 2 CO_2.
\end{align*}
\]

Different sets of kinetic rate equations are used for atmospheric conditions (case 1) and pressurized case (case 2). For the atmospheric conditions of case 1 the model for the effective reaction rates proposed by Vascellari et al. (2014) is used:

\[
\begin{align*}
rr_{R3,1} &= \theta(X) \cdot k_{a,1} \cdot \exp\left\{ -\frac{E_a}{R \cdot T} \right\} \cdot \frac{P_{CO_2}^n}{1 + K_{CO} \cdot P_{CO}}, \\
rr_{R4,1} &= \theta(X) \cdot k_{a,1} \cdot \exp\left\{ -\frac{E_a}{R \cdot T} \right\} \cdot \frac{P_{H2O}^m}{1 + K_{H_2} \cdot P_{H_2}}, \\
rr_{R5,1} &= \theta(X) \cdot k_{a,1} \cdot \exp\left\{ -\frac{E_a}{R \cdot T} \right\} \cdot \frac{P_{O_2}^p}{P_{O_2}}.
\end{align*}
\]

The rate constants are taken from Richter et al. (2016) and are given in Table 3. $\theta(X)$ is an empirical factor to account for the inner structure of the particle, which is calculated as described in Vascellari et al. (2014).
Table 3: Kinetic constants for the effective reaction rates of the boudouard, water gas and oxidation reactions from Richter et al. (2016).

<table>
<thead>
<tr>
<th>n</th>
<th>K/(1/ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R3</td>
<td>9.04⋅10^{-3}</td>
</tr>
<tr>
<td>R4</td>
<td>7.30</td>
</tr>
<tr>
<td>R5</td>
<td>1.77⋅10^{4}</td>
</tr>
</tbody>
</table>

At 30bar operating pressure (case 2), the intrinsic reaction rate data of Hla et al. (2007) is taken and modified with an effectiveness factor η_r to account for the transport resistances inside the particle. Hence the effective reaction rates are:

\[ r_{R3,2} = \eta_r P_{CO_2} \cdot S_V \cdot k_w \cdot \exp \left\{ -\frac{E_a}{R \cdot T} \right\} \cdot p_{CO_2}^{n_r} \]

\[ r_{R4,2} = \eta_r P_{H_2} \cdot S_V \cdot k_w \cdot \exp \left\{ -\frac{E_a}{R \cdot T} \right\} \cdot p_{H_2}^{n_r} \]

\[ r_{R5,2} = \eta_r P_{O_2} \cdot S_V \cdot k_w \cdot \exp \left\{ -\frac{E_a}{R \cdot T} \right\} \cdot p_{O_2}^{n_r} \]

The rate constants are given in Table 4.

Table 4: Kinetic constants for the intrinsic reaction rates of the boudouard, water gas and oxidation reactions fro Hla et al. (2007) for coal CRC272.

<table>
<thead>
<tr>
<th></th>
<th>k_w/(kmol/(m^3Pa^n))</th>
<th>E_a/(J/kmol)</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>R3</td>
<td>3.331⋅10^{-2}</td>
<td>2.11⋅10^{8}</td>
<td>0.4</td>
</tr>
<tr>
<td>R4</td>
<td>2.485</td>
<td>2.31⋅10^{8}</td>
<td>0.4</td>
</tr>
<tr>
<td>R5</td>
<td>1.236⋅10^{-3}</td>
<td>1.36⋅10^{8}</td>
<td>0.8</td>
</tr>
</tbody>
</table>

The effectivity for the species i and reaction j is estimated as

\[ \eta_{ij} = \frac{1}{\Phi_{ij}} \left( \frac{1}{\tanh[3\Phi_{ij}]} - \frac{1}{3\Phi_{ij}} \right) \]

using a generalized Thiele modules Φ_{ij} which is (almost) independent of the particle shape. For a power-law kinetic reaction rate defined it is defined as:

\[ \Phi_{ij} = \frac{V_p}{S_p} \sqrt{\frac{n + 1}{2} \cdot \frac{\lambda_{ij} \cdot k_w \cdot \exp \left\{ -\frac{E_a}{R \cdot T} \right\} \cdot S_V \cdot p_i^{n-1}}{D_{eff,i}}} \]

Simulation settings

ANSYS Fluent V 17.2 was used to solve the Navier-Stokes equations coupled with species and energy transport. The pressure based solver was used and the differential equations were discretized using second order schemes in space and time. Only the convective fluxes were discretized with a third-order MUSCL scheme in the steady RANS simulations. For the 2D-axisymmetric simulations the domain extends L_0 = 30d_p in upstream, L_1 = 100d_p in downstream and H = 40d_p in radial direction. Based on the 2D results, the 3D-domain has been chosen slightly smaller. The cuboid extends L_0 = 8d_p in upstream, L_1 = 24d_p in downstream and H = 8d_p in the lateral directions. The number of grid cells used is 27,750 for the 2D simulations and 4,085,112 for the 3D simulations. Grid-independence has been confirmed in previous investigations by Richter et al. (2015, 2016). A comprehensive validation of the model setup against different experimental data is given in Richter et al. (2013).

Results

In order to reduce the computational effort, as the final aim of this research is to study gasification in high detail with three-dimensional transient LES simulations, a semi-global mechanism is used in this work. Hence for comparison simulations have been done with the detailed drm22-mechanism proposed by Kazakov and Frenklach (1994). Results for the atmospheric case at Re = 500 are shown in Figure 2 and for the pressurized case at Re = 1000 in Figure 3. The general features of the flame structure are reproduced with the semi-global mechanism, however some differences can be observed in particular in the contours shown for the atmospheric case 1. The maximum temperature is higher and the high temperature zone is more pronounced for the semi-global mechanism. The maximum CO_2 mass fraction is larger when using the detailed mechanism, however the shape of the CO_2-rich zone is similar. The higher CO_2 mass fraction can be explained by the simplified semi-global mechanism, which only considers the hydrogen oxi-
dation R1 and the water-gas shift reaction R2, whereas the detailed DRM22 mechanism also includes the oxidation of CO to CO$_2$. Under the pressurized conditions of case 2 the differences in the results using the different mechanisms are less pronounced. Please note that the same gas phase mechanisms have been used in both cases, only the heterogeneous gas-surface reactions and the operating conditions are changed. The flame zone is slightly larger for the semi-global mechanism and the maximum temperature is slightly higher. Secondly the influence of turbulence on the gasification is studied. A qualitative comparison is presented in Figure 4, which shows the contours of the temperature for case 2 at different particle Reynolds-numbers. A similar picture is obtained for the atmospheric pressure case 1. The maximum temperature remains almost constant, however the shape and size of the flame zone significantly change with increasing particle Reynolds number. Fully engulfing the particle at low particle Reynolds numbers, the flame zone is gradually thinning with particle Reynolds number accompanied by an increasing fore-aft asymmetry such that a separated reaction zone persists at higher particle Reynolds numbers.

Quantitative data are given in Figures 5 and 6, which show the average temperature on the particle surface and the average carbon mass flux for case 1 and for case 2, respectively. Results are presented for 2D-axisymmetric RANS simulations and for 3D RANS simulations at the highest particle Reynolds number. The differences between the 2D and the 3D results are small, which shows that the 2D axisymmetric assumption is justified. Initially the eddy dissipation concept (EDC) model for turbulence-chemistry interaction has been used for all simulations with $Re > 200$. However in the graphs of the average surface temperature and also the species mass fractions a sudden jump has been found in the results rather than a smooth transition, which is considered non-physical. The red squares in the graphs for the surface temperature of Figures 5 and 6 show these findings. As the EDC model has originally been developed for highly turbulent flows, this model is considered the main suspect for the observed non-physical behaviour. Hence simulations with exactly the same simulations have been done, only with the turbulence-chemistry model turned off. The results are shown by the blue symbols in Figures 5 and 6. The jump has disappeared and a continuous change of surface temperature with particle Reynolds number can be seen. The contours of CO$_2$ mass fraction and temperature shown in Figure 7 for case 2 at $Re = 1000$ shed some lights on this question. Note that similar results are found for case 1 and for different particle Reynolds numbers. Qualitatively similar results are obtained for the simulations with and without turbulence-chemistry interaction turned on, only a higher temperatures and a higher CO$_2$ mass fraction are observed in the very thin flame zone close to the particle surface. However in this region the flow conditions are laminar and the grid is fine enough such that all scales are resolved. Hence the EDC model, which is based on the assumption of fully turbulent conditions, too strongly dampens the reactions which leads to the non-physical jump in the results. The carbon flux on the other hand is almost unaffected by the use of the EDC model and no clear jump is visible.

Finally, the dashed-lines in Figures 5 and 6 are a regression based on the laminar results, i.e. for $Re <= 200$. One sees that the extrapolation of the laminar results to higher particle Reynolds number still give a reasonable prediction of the carbon consumption, the maximum difference is about 10%.
CONCLUSIONS AND OUTLOOK

In this work the interplay between a turbulent chemically-reacting flow and heterogeneous gasification and combustion on a particle surface has been studied. It has been shown that the main features of the flame-zone are well captured using a simple semi-global gas phase mechanism and that the use of axisymmetric 2D simulations is justified. The use of the EDC turbulence-chemistry interaction leads to a too strong damping of the gas phase reactions near the particles, which strongly affects the surface temperature and species distribution, however the total carbon consumption rate is only mildly influenced. The reaction zone is strongly modified due to the change in wake structure. From engulfing the whole particle at low particle Reynolds numbers, a increasing fore-aft asymmetry has been found which lead to a separated flame zone at high particle Reynolds numbers. Despite the strong changes in the shape of the reaction zone, extrapolation of the laminar results into the turbulent regime gives a reasonable prediction of the carbon consumption rate and the surface temperature. This shows that models, based on laminar flow conditions, which are capable of capturing the fore-aft symmetry, can at least as a first estimate be used to also model gasification at larger particle Reynolds numbers. Finally as a completion of this work, currently 3D LES simulations are under way to study the effect of turbulent fluctuations on the overall carbon consumptions rate.

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