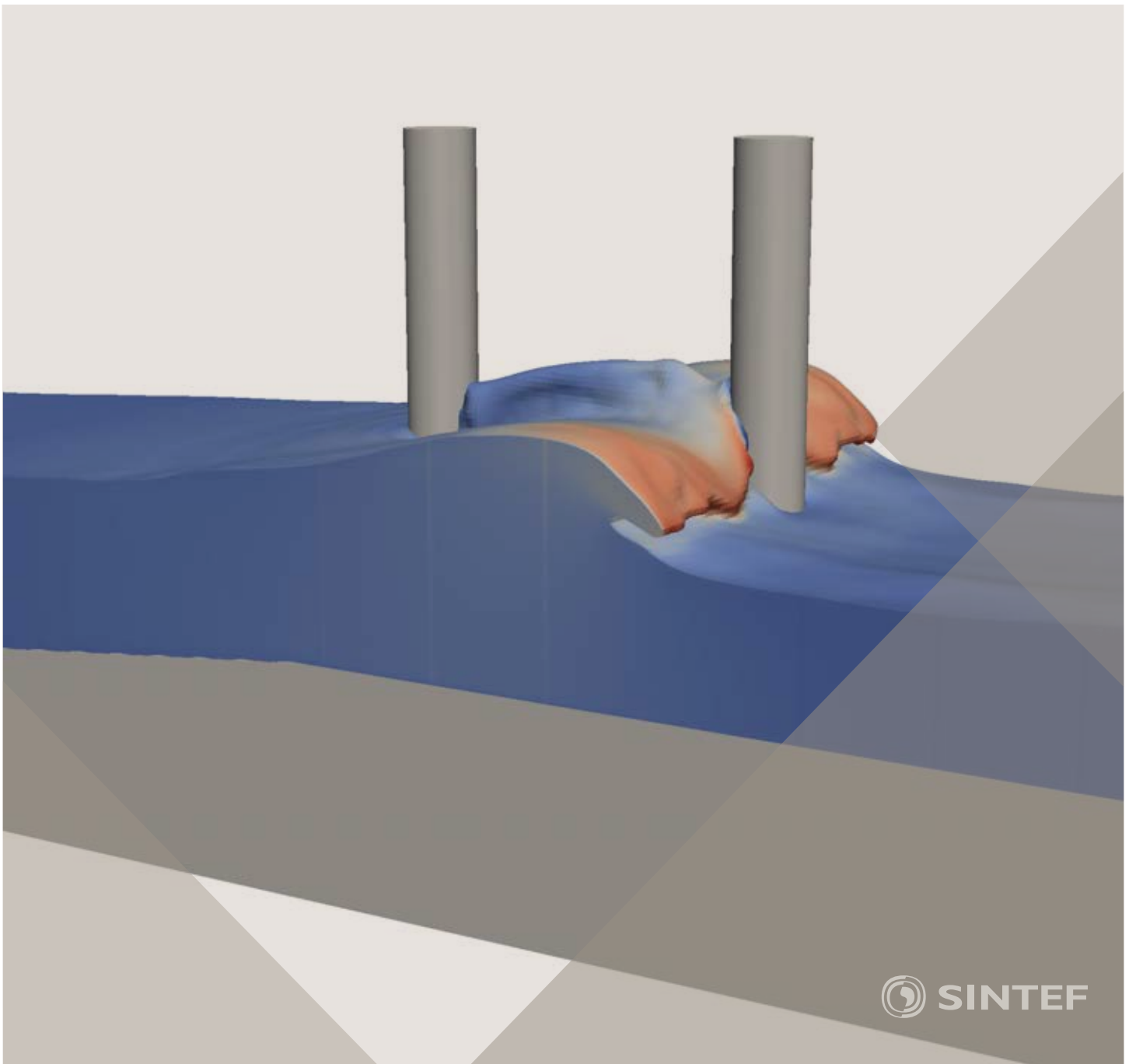


Proceedings of the 12<sup>th</sup> International Conference on  
Computational Fluid Dynamics in the Oil & Gas,  
Metallurgical and Process Industries

# Progress in Applied CFD – CFD2017



SINTEF Proceedings

Editors:

Jan Erik Olsen and Stein Tore Johansen

## **Progress in Applied CFD – CFD2017**

Proceedings of the 12<sup>th</sup> International Conference on Computational Fluid Dynamics  
in the Oil & Gas, Metallurgical and Process Industries

SINTEF Academic Press

SINTEF Proceedings no 2

Editors: Jan Erik Olsen and Stein Tore Johansen

**Progress in Applied CFD – CFD2017**

Selected papers from 10<sup>th</sup> International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Key words:

CFD, Flow, Modelling

Cover, illustration: Arun Kamath

ISSN 2387-4295 (online)

ISBN 978-82-536-1544-8 (pdf)

© Copyright SINTEF Academic Press 2017

The material in this publication is covered by the provisions of the Norwegian Copyright Act. Without any special agreement with SINTEF Academic Press, any copying and making available of the material is only allowed to the extent that this is permitted by law or allowed through an agreement with Kopinor, the Reproduction Rights Organisation for Norway. Any use contrary to legislation or an agreement may lead to a liability for damages and confiscation, and may be punished by fines or imprisonment

SINTEF Academic Press

Address:       Forskningsveien 3 B  
                  PO Box 124 Blindern  
                  N-0314 OSLO

Tel:             +47 73 59 30 00

Fax:            +47 22 96 55 08

[www.sintef.no/byggforsk](http://www.sintef.no/byggforsk)

[www.sintefbok.no](http://www.sintefbok.no)

**SINTEF Proceedings**

SINTEF Proceedings is a serial publication for peer-reviewed conference proceedings on a variety of scientific topics.

The processes of peer-reviewing of papers published in SINTEF Proceedings are administered by the conference organizers and proceedings editors. Detailed procedures will vary according to custom and practice in each scientific community.

## 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 focuses 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.

Stein Tore Johansen & Jan Erik Olsen



Organizing committee:

Conference chairman: Prof. Stein Tore Johansen

Conference coordinator: Dr. Jan Erik Olsen

Dr. Bernhard Müller

Dr. Sigrid Karstad Dahl

Dr. Shahriar Amini

Dr. Ernst Meese

Dr. Josip Zoric

Dr. Jannike Solsvik

Dr. Peter Witt

Scientific committee:

Stein Tore Johansen, SINTEF/NTNU

Bernhard Müller, NTNU

Phil Schwarz, CSIRO

Akio Tomiyama, Kobe University

Hans Kuipers, Eindhoven University of Technology

Jinghai Li, Chinese Academy of Science

Markus Braun, Ansys

Simon Lo, CD-adapco

Patrick Segers, Universiteit Gent

Jiyuan Tu, RMIT

Jos Derksen, University of Aberdeen

Dmitry Eskin, Schlumberger-Doll Research

Pär Jönsson, KTH

Stefan Pirker, Johannes Kepler University

Josip Zoric, SINTEF

## CONTENTS

<b>PRAGMATIC MODELLING .....</b>	<b>9</b>
On pragmatism in industrial modeling. Part III: Application to operational drilling .....	11
CFD modeling of dynamic emulsion stability .....	23
Modelling of interaction between turbines and terrain wakes using pragmatic approach .....	29
<b>FLUIDIZED BED .....</b>	<b>37</b>
Simulation of chemical looping combustion process in a double looping fluidized bed reactor with cu-based oxygen carriers.....	39
Extremely fast simulations of heat transfer in fluidized beds.....	47
Mass transfer phenomena in fluidized beds with horizontally immersed membranes .....	53
A Two-Fluid model study of hydrogen production via water gas shift in fluidized bed membrane reactors .....	63
Effect of lift force on dense gas-fluidized beds of non-spherical particles .....	71
Experimental and numerical investigation of a bubbling dense gas-solid fluidized bed .....	81
Direct numerical simulation of the effective drag in gas-liquid-solid systems .....	89
A Lagrangian-Eulerian hybrid model for the simulation of direct reduction of iron ore in fluidized beds.....	97
High temperature fluidization - influence of inter-particle forces on fluidization behavior .....	107
Verification of filtered two fluid models for reactive gas-solid flows .....	115
<b>BIOMECHANICS.....</b>	<b>123</b>
A computational framework involving CFD and data mining tools for analyzing disease in carotid artery .....	125
Investigating the numerical parameter space for a stenosed patient-specific internal carotid artery model.....	133
Velocity profiles in a 2D model of the left ventricular outflow tract, pathological case study using PIV and CFD modeling.....	139
Oscillatory flow and mass transport in a coronary artery.....	147
Patient specific numerical simulation of flow in the human upper airways for assessing the effect of nasal surgery.....	153
CFD simulations of turbulent flow in the human upper airways .....	163
<b>OIL &amp; GAS APPLICATIONS .....</b>	<b>169</b>
Estimation of flow rates and parameters in two-phase stratified and slug flow by an ensemble Kalman filter .....	171
Direct numerical simulation of proppant transport in a narrow channel for hydraulic fracturing application .....	179
Multiphase direct numerical simulations (DNS) of oil-water flows through homogeneous porous rocks .....	185
CFD erosion modelling of blind tees .....	191
Shape factors inclusion in a one-dimensional, transient two-fluid model for stratified and slug flow simulations in pipes .....	201
Gas-liquid two-phase flow behavior in terrain-inclined pipelines for wet natural gas transportation .....	207

<b>NUMERICS, METHODS &amp; CODE DEVELOPMENT .....</b>	<b>213</b>
Innovative computing for industrially-relevant multiphase flows .....	215
Development of GPU parallel multiphase flow solver for turbulent slurry flows in cyclone.....	223
Immersed boundary method for the compressible Navier–Stokes equations using high order summation-by-parts difference operators .....	233
Direct numerical simulation of coupled heat and mass transfer in fluid-solid systems .....	243
A simulation concept for generic simulation of multi-material flow, using staggered Cartesian grids.....	253
A cartesian cut-cell method, based on formal volume averaging of mass, momentum equations.....	265
SOFT: a framework for semantic interoperability of scientific software .....	273
 <b>POPULATION BALANCE .....</b>	 <b>279</b>
Combined multifluid-population balance method for polydisperse multiphase flows .....	281
A multifluid-PBE model for a slurry bubble column with bubble size dependent velocity, weight fractions and temperature.....	285
CFD simulation of the droplet size distribution of liquid-liquid emulsions in stirred tank reactors .....	295
Towards a CFD model for boiling flows: validation of QMOM predictions with TOPFLOW experiments .....	301
Numerical simulations of turbulent liquid-liquid dispersions with quadrature-based moment methods.....	309
Simulation of dispersion of immiscible fluids in a turbulent couette flow .....	317
Simulation of gas-liquid flows in separators - a Lagrangian approach.....	325
CFD modelling to predict mass transfer in pulsed sieve plate extraction columns .....	335
 <b>BREAKUP &amp; COALESCENCE .....</b>	 <b>343</b>
Experimental and numerical study on single droplet breakage in turbulent flow .....	345
Improved collision modelling for liquid metal droplets in a copper slag cleaning process .....	355
Modelling of bubble dynamics in slag during its hot stage engineering.....	365
Controlled coalescence with local front reconstruction method .....	373
 <b>BUBBLY FLOWS .....</b>	 <b>381</b>
Modelling of fluid dynamics, mass transfer and chemical reaction in bubbly flows .....	383
Stochastic DSMC model for large scale dense bubbly flows.....	391
On the surfacing mechanism of bubble plumes from subsea gas release.....	399
Bubble generated turbulence in two fluid simulation of bubbly flow .....	405
 <b>HEAT TRANSFER .....</b>	 <b>413</b>
CFD-simulation of boiling in a heated pipe including flow pattern transitions using a multi-field concept .....	415
The pear-shaped fate of an ice melting front .....	423
Flow dynamics studies for flexible operation of continuous casters (flow flex cc).....	431
An Euler-Euler model for gas-liquid flows in a coil wound heat exchanger.....	441
 <b>NON-NEWTONIAN FLOWS.....</b>	 <b>449</b>
Viscoelastic flow simulations in disordered porous media .....	451
Tire rubber extrudate swell simulation and verification with experiments .....	459
Front-tracking simulations of bubbles rising in non-Newtonian fluids.....	469
A 2D sediment bed morphodynamics model for turbulent, non-Newtonian, particle-loaded flows.....	479

<b>METALLURGICAL APPLICATIONS.....</b>	<b>491</b>
Experimental modelling of metallurgical processes .....	493
State of the art: macroscopic modelling approaches for the description of multiphysics phenomena within the electroslag remelting process .....	499
LES-VOF simulation of turbulent interfacial flow in the continuous casting mold .....	507
CFD-DEM modelling of blast furnace tapping .....	515
Multiphase flow modelling of furnace tapholes .....	521
Numerical predictions of the shape and size of the raceway zone in a blast furnace.....	531
Modelling and measurements in the aluminium industry - Where are the obstacles? .....	541
Modelling of chemical reactions in metallurgical processes.....	549
Using CFD analysis to optimise top submerged lance furnace geometries .....	555
Numerical analysis of the temperature distribution in a martensitic stainless steel strip during hardening.....	565
Validation of a rapid slag viscosity measurement by CFD.....	575
Solidification modeling with user defined function in ANSYS Fluent.....	583
Cleaning of polycyclic aromatic hydrocarbons (PAH) obtained from ferroalloys plant.....	587
Granular flow described by fictitious fluids: a suitable methodology for process simulations .....	593
A multiscale numerical approach of the dripping slag in the coke bed zone of a pilot scale Si-Mn furnace.....	599
<b>INDUSTRIAL APPLICATIONS .....</b>	<b>605</b>
Use of CFD as a design tool for a phosphoric acid plant cooling pond .....	607
Numerical evaluation of co-firing solid recovered fuel with petroleum coke in a cement rotary kiln: Influence of fuel moisture .....	613
Experimental and CFD investigation of fractal distributor on a novel plate and frame ion-exchanger .....	621
<b>COMBUSTION .....</b>	<b>631</b>
CFD modeling of a commercial-size circle-draft biomass gasifier.....	633
Numerical study of coal particle gasification up to Reynolds numbers of 1000.....	641
Modelling combustion of pulverized coal and alternative carbon materials in the blast furnace raceway .....	647
Combustion chamber scaling for energy recovery from furnace process gas: waste to value .....	657
<b>PACKED BED.....</b>	<b>665</b>
Comparison of particle-resolved direct numerical simulation and 1D modelling of catalytic reactions in a packed bed .....	667
Numerical investigation of particle types influence on packed bed adsorber behaviour .....	675
CFD based study of dense medium drum separation processes .....	683
A multi-domain 1D particle-reactor model for packed bed reactor applications.....	689
<b>SPECIES TRANSPORT &amp; INTERFACES .....</b>	<b>699</b>
Modelling and numerical simulation of surface active species transport - reaction in welding processes .....	701
Multiscale approach to fully resolved boundary layers using adaptive grids.....	709
Implementation, demonstration and validation of a user-defined wall function for direct precipitation fouling in Ansys Fluent.....	717



<b>FREE SURFACE FLOW &amp; WAVES .....</b>	<b>727</b>
Unresolved CFD-DEM in environmental engineering: submarine slope stability and other applications.....	729
Influence of the upstream cylinder and wave breaking point on the breaking wave forces on the downstream cylinder .....	735
Recent developments for the computation of the necessary submergence of pump intakes with free surfaces .....	743
Parallel multiphase flow software for solving the Navier-Stokes equations .....	752
<b>PARTICLE METHODS .....</b>	<b>759</b>
A numerical approach to model aggregate restructuring in shear flow using DEM in Lattice-Boltzmann simulations .....	761
Adaptive coarse-graining for large-scale DEM simulations.....	773
Novel efficient hybrid-DEM collision integration scheme.....	779
Implementing the kinetic theory of granular flows into the Lagrangian dense discrete phase model.....	785
Importance of the different fluid forces on particle dispersion in fluid phase resonance mixers .....	791
Large scale modelling of bubble formation and growth in a supersaturated liquid.....	798
<b>FUNDAMENTAL FLUID DYNAMICS .....</b>	<b>807</b>
Flow past a yawed cylinder of finite length using a fictitious domain method .....	809
A numerical evaluation of the effect of the electro-magnetic force on bubble flow in aluminium smelting process.....	819
A DNS study of droplet spreading and penetration on a porous medium.....	825
From linear to nonlinear: Transient growth in confined magnetohydrodynamic flows.....	831

## A LAGRANGIAN-EULERIAN HYBRID MODEL FOR THE SIMULATION OF DIRECT REDUCTION OF IRON ORE IN FLUIDIZED BEDS

Simon SCHNEIDERBAUER<sup>1\*</sup>, Mustafa E. KINACI<sup>1†</sup>, Franz HAUZENBERGER<sup>2‡</sup>, Stefan PIRKER<sup>3§</sup>

<sup>1</sup>Christian-Doppler Laboratory for Multi-Scale Modelling of Multiphase Processes, Johannes Kepler University, 4040 Linz, AUSTRIA

<sup>2</sup>Primetals Technologies Austria GmbH, 4031 Linz, AUSTRIA

<sup>3</sup>Department of Particulate Flow Modelling, Johannes Kepler University, 4040 Linz, AUSTRIA

\* E-mail: simon.schneiderbauer@jku.at

† E-mail: mustafa\_efe.kinaci@jku.at

‡ E-mail: franz.hauzenberger@primetals.com

§ E-mail: stefan.pirker@jku.at

### ABSTRACT

Fluidized bed and moving bed reactors are one of the most important technologies in several branches of process industry. Especially, it is known since decades that iron can be reduced rapidly and efficiently from iron carrier materials using such. The primary energy sources and reducing agents are natural gas, coal, coke, pulverized coal, which are finally released as CO<sub>2</sub> and in a lesser extent as H<sub>2</sub>O to the environment. Iron reduction consumes about 70% of the energy during steelmaking therefore offering potential in energy and CO<sub>2</sub> savings. Due to the limited accessibility for measurements, simulation methods have become one of the most important tools for optimizing the iron making processes. While the two-fluid model (Schneiderbauer *et al.*, 2012) would be a good candidate to attack the simulation of large-scale multi-phase processes it lacks from a proper representation of the particle size distribution and the related physical phenomena. This, in turn, gives rise to particle-based approaches, such as the coupling between CFD and DEM methods, which can easily handle particle segregation, particle growth and particle mixing. Furthermore, chemical reactions can be evaluated per particle and it is not required to transfer these reactions to a continuum representation. However, CFD-DEM approaches require an appropriate coarse-graining to considerably reduce their computational demands. We, therefore, present a generalization of the Lagrangian-Eulerian hybrid model for the numerical assessment of reacting poly-disperse gas-solid flows (Schneiderbauer *et al.*, 2016b) to fluidized beds used for iron ore reduction. The main idea of such a modeling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and a coarse-grained two-fluid model (TFM) to take advantage of the benefits of those two different formulations. On the one hand, the DPM model unveils additional information such as the local particle size distribution, which is not covered by TFM. On the other hand, the TFM solution deflects the DPM trajectories due to the inter-particle stresses. This hybrid approach further enables the efficient evaluation of the gas-solid phase reduction of iron ore at a particle level using DPM. The predictive capability and numerical efficiency of this reactive hybrid modeling approach is demonstrated in the case of a lab-scale fluidized bed. The results show that the model is able to correctly predict fractional reduction of the iron ore. The results further give a closer insight about the temperatures and reaction gas consumption due to the reduction process.

**Keywords:** fluidized bed, iron ore reduction, two-fluid model.

A complete list of symbols used, with dimensions, is re-

quired.

### NOMENCLATURE

#### Greek Symbols

$\beta$	drag coefficient, [ $kg/m^3s$ ]
$\rho$	Mass density, [ $kg/m^3$ ]
$\epsilon$	volume fraction, (-)
$\mu_g$	viscosity of gas phase, [ $Pa s$ ]
$\tau$	Tortuosity, (-)

#### Latin Symbols

$a, b, c$  Stoichiometric coefficients of relative species

$A, B, C$  Species

$A_p$	Particle surface area, [ $m^2$ ]
$C_i$	Molar Concentration of species $i$ , [ $mol/m^3$ ]
$D_{j,i}$	Binary gas diffusion, [ $m^2/s$ ]
$d$	Particle diameter, [ $m$ ]
$E_a$	Activation energy, [ $kJ/mol$ ]
$f_j$	Local fractional reduction of the $j^{th}$ layer, [ $kJ/mol$ ]
$G_\Delta$	Box filter defined by numerical grid, (-)
$k_0$	Pre-exponential factor, [ $m/s$ ]
$Ke_j$	Equilibrium constant of layer $j$ , (-)
$k_f$	Mass transfer coefficient, [ $m/s$ ]
$k_j$	Reaction rate constant, [ $m/s$ ]
$m_i$	Mass of species $i$ , [ $kg$ ]
$M_i$	Molecular mass of species $i$ , [ $kg/mol$ ]
$N_i$	Number of moles of species $i$ , [ $mol$ ]
$n$	Number density, [ $1/m^3$ ]
$Nu$	Nusselt number, (-)
$Pr$	Prandtl number, (-)
$P_t$	Total pressure, [ $bar$ ]
$R$	Universal gas constant, [ $kJ/molK$ ]
$Re$	Reynolds number, (-)
$r_p$	Particle radius, [ $m$ ]
$r_j$	Layer radius, [ $m$ ]
$Sc$	Schmidt number, (-)
$Sh$	Sherwood number, (-)
$T$	Temperature, [ $K$ ]
$u$	velocity, [ $m/s$ ]
$\dot{Y}_{i,j}$	Mass fraction of species $i$ layer $j$ , (-)
$X_i$	Molar fraction of species $i$ , (-)

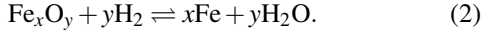
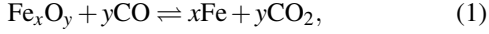
#### Sub/superscripts

$g$	Gas phase
$i$	species $i$
$j$	layer $j$

s solid phase

## INTRODUCTION

The main conversion process to gain metallic iron from oxidic iron compounds is the reduction of iron ores by suitable reducing agents, where iron oxides are reduced to metallic iron by gaseous reducing agents (CO and H<sub>2</sub>). During the reduction of iron ores, oxygen is removed according to the thermodynamic equilibrium conditions, until the next oxidation level is reached. The gaseous reduction of iron oxides as well as the oxidation of the reducing agents can be described by the following reaction mechanism (Valipour, 2009)



These equations reveal that the reduction reactions of iron ores can be considered as elementary reactions, which means that the number of moles of the gaseous components does not change during the reactions. Thus, the equilibrium of reactions is independent of the total pressure of the reaction system and the chemical equilibrium conditions only depend on temperature.

The leading process used in iron-making is the blast furnace, which consists of a moving bed reactor with countercurrent flow of the solid reactants against a reducing gas. In the lower part the iron is molten and carburized. However, in the blast furnace process iron ore fines, which build up around 80% of the total iron ore, needs to go through a preparation step (i.e. pelletizing or sintering process; Schenk (2011)). In contrast, by using fluidized bed technology fine ores can directly be charged into the reduction process. Such fluidized bed reactors are used, for example, in the FINEX<sup>®</sup> process (Habermann *et al.*, 2000; Primetals Technologies Austria GmbH and POSCO E&C, 2015). The FINEX<sup>®</sup> process, which was jointly developed by POSCO (Korea) and Primetals Technologies (Austria), produces hot metal in the same quality as traditional blast furnaces, however the coke making and sintering of the fine ores are avoided. The iron-ores that are charged into the process go through fluidized bed reactors where they are heated and reduced to DRI (Direct Reduced Iron), charged into the melter gasifier, where final reduction and melting as well as the production of reducing gas by gasification of coal with oxygen takes place (Plaul *et al.*, 2009).

Due to the limited accessibility for measurements, simulation methods have become one of the most important tools for optimizing the iron making processes (Valipour, 2009; Natsui *et al.*, 2014; Valipour *et al.*, 2006; Fu *et al.*, 2014). However, either these numerical models neglect the impact of the reduction of iron ore (Fu *et al.*, 2014) or these are restricted to very small scale processes such as, individual pellets (Valipour, 2009; Valipour *et al.*, 2006) or lab-scale fluidized beds (Natsui *et al.*, 2014). It has to be noted that the latter utilized the CFD-DEM approach to model the gas-solid flow, where the continuous phase is governed by computational fluid dynamics (CFD) and the particle trajectories are computed by using the discrete element method (DEM), which is rather computationally demanding (Goniva *et al.*, 2012).

Since the total number of particles in fluidized bed reactors is extremely large, it may be impractical to solve the equations of motion for each particle. It is, therefore, common to investigate particulate flows in large process units using averaged equations of motion, i.e. two-fluid models (TFM),

which include the inter-particle collisions statistically by kinetic theory based closures of the particle stresses (Lun *et al.*, 1984; Schneiderbauer *et al.*, 2012; Agrawal *et al.*, 2001). However, each representative particle diameter requires an additional momentum and continuity equation, which considerably raises the computational demand with increasing number of particle diameters (Iddir and Arastoopour, 2005; Schellander *et al.*, 2013). One may restrict the calculations to spatially constant particle size distributions to evaluate the gas-solid drag force (Schneiderbauer *et al.*, 2015a). To overcome this deficiency of TFM, we follow our previous work (Schneiderbauer *et al.*, 2016a; Schellander *et al.*, 2013; Pirker *et al.*, 2010; Schneiderbauer *et al.*, 2015b; Pirker and Kahrmanovic, 2009) and employ a hybrid model for the numerical assessment of poly-disperse gas-solid fluidized beds. The main idea of such a modeling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and a TFM to take advantage of the benefits of those two different formulations. On the one hand, the local degree of poly-dispersity (i.e. the local particle size distribution), which is essential for the evaluation of the gas-solid drag force, can be obtained by tracking statistically representative particle trajectories for each particle diameter class. On the other hand, the computationally demanding tracking of the inter-particle collisions can be obtained from the inter-particle stresses, which are deduced from the TFM solution. These then appear in addition to the gas-particle drag as a body force in the equation of motion of each DPM-trajectory. Thus, the hybrid model represents a TFM simulation with additional DPM particles, which are used, for example, to provide a closure for the poly-disperse drag law. Finally, by employing the above Lagrangian-Eulerian hybrid model, the reduction of the iron ore as well as the corresponding reaction heat can be computed based on the representative Lagrangian particles. This, in turn, includes the conversion of iron oxides to iron.

In this paper, we employ a Eulerian-Lagrangian hybrid model (Schneiderbauer *et al.*, 2016a,b) to the direct reduction of iron ore in fluidized beds. Here, the reduction is computed based on representative Lagrangian trajectories, where the reduction model is based on literature (Hanel *et al.*, 2015; Valipour, 2009; Valipour *et al.*, 2006; Natsui *et al.*, 2014).

## POLY-DISPERSE GAS-SOLID FLOWS

### Two-fluid model (TFM)

In this work, we used a kinetic-theory based two-fluid model (TFM) to study fluidized beds. Since these equations have been extensively discussed in our previous work (Schneiderbauer *et al.*, 2013, 2012; Schneiderbauer and Pirker, 2014), we do not repeat all the details here and solely present the continuity and momentum equations for the solid phase below:

$$\frac{\partial}{\partial t} \varepsilon_s \rho_s + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = \mathcal{R}_s, \quad (3)$$

$$\frac{\partial}{\partial t} (\varepsilon_s \rho_s \mathbf{u}_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) = -\varepsilon_s \nabla p - \nabla \cdot (\boldsymbol{\Sigma}_s^{\text{kc}} + \boldsymbol{\Sigma}_s^{\text{fir}}) + \beta (\mathbf{u}_g - \mathbf{u}_s) + \varepsilon_s \rho_s \mathbf{g}. \quad (4)$$

Here,  $\rho_s$ ,  $\varepsilon_s$  and  $\mathbf{u}_s$  denote density, volume fraction and local-average velocity of the solid phase, respectively;  $\mathcal{R}_s$  denotes the rate of oxygen removal due to chemical reactions;  $p$  is the gas phase pressure;  $\mathbf{u}_g$  is the local-average velocity of the gas phase;  $\beta$  is the microscopic drag coefficient, which is closed by the poly-disperse drag law of Beetstra *et al.* (2007) (see

table 1);  $\mathbf{g}$  is the gravitational acceleration; finally,  $\Sigma_s^{\text{kc}}$  and  $\Sigma_s^{\text{fr}}$  are the stress tensors associated with the solids phase, where the frictional contribution,  $\Sigma_s^{\text{fr}}$ , arises from enduring or multi-particle collision events in dense areas. The kinetic-collisional part,  $\Sigma_s^{\text{kc}}$ , is closed using kinetic theory (Hrenya and Sinclair, 1997; Lun *et al.*, 1984), which requires an additional equation for the granular temperature. It has to be further noted that in our previous study (Schellander *et al.*, 2013) we considered an additional term on the right hand side of the solids momentum equation, which accounted for the impact of particle rotation (Magnus force). Particle rotation is assumed to be non-significant in fluidized beds and is therefore included in this work.

### Lagrangian discrete phase model (DPM)

We follow our previous work (Schneiderbauer *et al.*, 2016a,b) and obtain the local volume fraction of the different particle size classes  $\varepsilon_{s,i} = x_i \varepsilon_s$ , which is required for the evaluation of the gas-solid drag force (compare with table 1), by tracking statistically representative particle trajectories for each particle diameter class along the solids flow obtained from TFM. In particular, such a trajectory  $k$  represents  $a_k$  real particles, which are referred to parcels (Radl and Sundaresan, 2014). Thus, we obtain for the number density of size class  $i$

$$n_i(\mathbf{x}) = \sum_{k \in \mathcal{P}_i} a_k G_{\Delta_g}(\mathbf{x} - \mathbf{x}_{p,k}), \quad (5)$$

which is connected to the volume fraction  $\varepsilon_{s,i}$  by

$$\varepsilon_{s,i} = n_i \pi \frac{d_{s,i}^3}{6} \quad (6)$$

yielding

$$x_i = \pi \frac{d_{s,i}^3}{6} \frac{n_i}{\varepsilon_s} \quad (7)$$

In equation (5),  $\Delta_g$  denotes the grid spacing of the Eulerian grid and the set  $\mathcal{P}_i$  contains all parcels of particle size class  $i$ . We further obtain the local Sauter diameter, which is required for the evaluation of the drag force and the kinetic theory stresses, from

$$\langle d_s \rangle = \left[ \sum_{i=1}^{N_{sp}} \frac{x_i}{d_{s,i}} \right]^{-1}, \quad (8)$$

where  $N_{sp}$  the number of particle size classes.

It remains to discuss the equation of motion of such a tracer parcel  $k$ , which reads (Schneiderbauer *et al.*, 2016a, 2015b)

$$\frac{d\mathbf{u}_{p,k}}{dt} = \frac{1}{\tau_{c,k}} (\mathbf{u}_s - \mathbf{u}_{p,k}) + \mathbf{F}_k^{\text{poly}} + \mathbf{g}, \quad (9)$$

where  $\mathbf{u}_{p,k}$  denotes the velocity of the Lagrangian tracer parcel  $k$ ,  $\mathbf{u}_s$  the solids velocity,  $\mathbf{g}$  the gravitational acceleration and  $\tau_{c,k}$  is a collisional time scale required to accelerate a single particle to the average solids velocity (Syamlal *et al.*, 1993; Schneiderbauer *et al.*, 2016a, 2015b)

$$\frac{1}{\tau_{c,k}} = \frac{3(1+e)}{4} \varepsilon_s \|\mathbf{u}_{p,k} - \mathbf{u}_s\| \sum_j^{N_{sp}} \frac{x_j (d_{s,k} + d_{s,j})^2 g_{0,kj}}{d_{s,k}^3 + d_{s,j}^3}. \quad (10)$$

Here,  $e \approx 0.9$  is the coefficient of restitution,  $N_{sp}$  is defined in equation (8),  $d_{s,j}$  the particle diameter of class  $j$  and  $x_j$  is

defined in table 1.  $g_{0,jk}$  denotes the radial distribution function, which accounts for the poly-disperse mixture of hard spheres (Iddir and Arastoopour, 2005). Note that equation (10) accounts for the contribution coming from the inter-particle stresses, i.e. inter-particle collisions. These are determined by the coarse-grained TFM solution and affect the trajectories of the tracer parcels by the collisional time scale  $\tau_{c,k}$ .

Since the tracers show different particle diameters  $\mathbf{F}_k^{\text{poly}}$  is the acceleration of a single particle of diameter  $d_{s,k}$  within the local poly-disperse mixture of particles (units force per unit parcel mass, i.e.  $\text{m s}^{-2}$ ) due to the gas-solid drag force. Thus, the acceleration of parcel  $k$  due to the drag force can be written as (Schneiderbauer *et al.*, 2016a)

$$\mathbf{F}_k^{\text{poly}} = \frac{1}{x_k \varepsilon_s \rho_s} \beta_k (\mathbf{u}_g - \mathbf{u}_{p,k}), \quad (11)$$

where  $\tilde{\beta}_k$  is presented in table 1. Note that here  $\beta_k$  is computed based on the Reynolds number computed from the local velocity of the tracer instead of the local velocity of the solid phase.

### DIRECT REDUCTION OF IRON ORE

In the following, we briefly present the reduction model. For more details the reader is referred to Kinaci *et al.* (2017).

### Species Transport and Heat Transfer

The local concentration of the reactant  $i$  is described by a transport equation for a corresponding species  $Y_i$  of the gas phase, which reads

$$\frac{\partial \varepsilon_g \rho_g Y_i}{\partial t} + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g Y_i) = -\nabla \varepsilon_g \mathbf{J}_i + \varepsilon_g \mathcal{R}_i, \quad (12)$$

where  $\rho_g$  is the density of the gas phase given by the equation of state for ideal gases and  $\mathcal{R}_i$  accounts for net rate of generation/destruction of species  $i$  by chemical reactions. Finally, the diffusion flux  $\mathbf{J}_i$  is written as

$$\mathbf{J}_i = -\rho_g D_{m,i} \nabla Y_i - D_{T,i} \frac{\nabla T_g}{T_g}, \quad (13)$$

where  $D_{m,i}$  is the mass diffusion coefficient for species  $i$  and  $D_{T,i}$  is the thermal (Soret) diffusion coefficient (ANSYS, 2011).

To describe the conservation of energy in fluidized bed reactors, a separate transport equation is solved for the specific enthalpy,  $h_q$ , of each phase:

$$\frac{\partial \varepsilon_q \rho_q h_q}{\partial t} + \nabla \cdot (\varepsilon_q \rho_q \mathbf{u}_q h_q) = \Sigma_q : \nabla \mathbf{u}_q - \nabla \cdot \mathbf{q}_q + S_q + Q_{gs}, \quad (14)$$

where the heat flux  $\mathbf{q}_q$  is modeled by using Fourier's law  $\mathbf{q}_q = k_q \nabla T_q$  and  $S_q$  accounts for the reaction heat. In case of the gas phase the heat conductivity  $k_g$  is computed employing a weighted average of the individual heat conductivities of the monomers. For the heat exchange between the gas and the solid phase,  $Q_{gs}$ , we employ the correlation proposed by Gunn (1978). Assuming constant specific heats  $c_{p,q}$  the phase temperature and phase enthalpy are correlated as follows

$$h_q = c_{p,q} T_q. \quad (15)$$

**Table 1:** Summary of microscopic poly-disperse drag coefficient of Beetstra *et al.* (2007), which has been adapted in our previous work (Schneiderbauer *et al.*, 2015a). Here,  $\bar{\epsilon}_g$  denotes the filtered gas volume fraction,  $\langle d_s \rangle$  the Sauter diameter,  $\epsilon_{s,i}$  the volume fraction of particle size class  $i$  and  $N_{sp}$  the number of particle size classes.

$$\tilde{\beta} = 18\mu_g \bar{\epsilon}_s \bar{\epsilon}_g^2 F(\bar{\epsilon}_s, \bar{\epsilon}_g, \widetilde{\text{Re}}_{\langle d_s \rangle}) \left( \sum_{i=1}^{N_{sp}} \bar{x}_i F_{\text{poly}}(y_i) \right),$$

with

$$\begin{aligned} \widetilde{\text{Re}}_{\langle d_s \rangle} &= \frac{\bar{\epsilon}_g \rho_g \langle d_s \rangle \|\tilde{\mathbf{u}}_g - \tilde{\mathbf{u}}_s\|}{\mu_g}, \\ F_{\text{poly}}(y_i) &= \bar{\epsilon}_g y_i + \bar{\epsilon}_s y_i^2 + 0.064 \bar{\epsilon}_g y_i^3, \\ F(\bar{\epsilon}_s, \bar{\epsilon}_g, \widetilde{\text{Re}}_{\langle d_s \rangle}) &= \frac{10\bar{\epsilon}_s}{\bar{\epsilon}_g^3} + \bar{\epsilon}_g (1 + 1.5\bar{\epsilon}_s^{1/2}) + \frac{0.413 \widetilde{\text{Re}}_{\langle d_s \rangle}}{24\bar{\epsilon}_g^3} \left( \frac{\bar{\epsilon}_g^{-1} + 3\bar{\epsilon}_g \bar{\epsilon}_s + 8.4 \widetilde{\text{Re}}_{\langle d_s \rangle}^{-0.343}}{1 + 10^{3\bar{\epsilon}_s} \widetilde{\text{Re}}_{\langle d_s \rangle}^{-(1+4\bar{\epsilon}_s)/2}} \right) \end{aligned}$$

and the dimensionless parameters

$$\bar{x}_i = \frac{\bar{\epsilon}_{s,i}}{\bar{\epsilon}_s}, \quad y_i = \frac{d_i}{\langle d_s \rangle}$$

## Thermochemical Aspects

Modelling direct reduction of iron ore can be related to equilibrium phase diagrams. One such diagram demonstrates the reduction processes of the iron-oxygen-carbon system, which is also called the *Baur-Glaessner Diagram*. In this diagram, the stabilities for the iron-oxides and iron phases are depicted as a function of temperature and CO/CO<sub>2</sub> (H<sub>2</sub>/H<sub>2</sub>O) mixture with the available correlations for the equilibrium constant from literature and the ones calculated.

The concentration molar fraction of the relative gas species can be determined with the use of the equilibrium constant as

$$\frac{x_{\text{CO}_2}}{x_{\text{CO}}} = K e_{\text{Fe}_x\text{O}_y, \text{CO}}, \quad (16)$$

thus the molar fraction of the mixture can be defined with,

$$x_{\text{CO}_2} = k_c \frac{K e_{\text{Fe}_x\text{O}_y, \text{CO}}}{1 + K e_{\text{Fe}_x\text{O}_y, \text{CO}}} \quad (17)$$

or

$$x_{\text{CO}} = k_c \frac{1}{1 + K e_{\text{Fe}_x\text{O}_y, \text{CO}}}, \quad (18)$$

in which  $k_c$  represents the total content of carbon in the system that can be expressed with

$$x_{\text{CO}} + x_{\text{CO}_2} = k_c. \quad (19)$$

As a more advanced method one might consider a four-component gas mixture of CO, H<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O to be represented in a single Baur-Glaessner Diagram with an abscissa of CO + H<sub>2</sub> or H<sub>2</sub>O + CO<sub>2</sub> content.

## Reaction Kinetics

The most common types of representation models for the non-catalytic reactions of solids submerged in fluids is the shrinking particle model (SPM) and the unreacted shrinking core model (USCM) (Levenspiel, 1999), where the unreacted shrinking core model is accepted as the most precise model to represent direct reduction of iron ore (Valipour *et al.*, 2006; Valipour, 2009; Natsui *et al.*, 2014). In particular, the three layer unreacted shrinking core model developed by Philbrook, Spitzer and Manning (Tsay *et al.*, 1976) is able

to represent the three interfaces of hematite/magnetite, magnetite/wustite and wustite/iron. For further details about the current implementation of the USCM the reader is referred to Kinaci *et al.* (2017).

According to Tsay *et al.* (1976) the removal rate of oxygen is determined through the following mechanisms: (i) The reducing gas is transported through the gas film onto the particle surface ( $F$ ); (ii) diffusion through the porous iron layer ( $B_3$ ); (iii) reactants react with wustite at the wustite/iron interface and form iron ( $A_3$ ); (iv) remaining reactants diffuse through the wustite layer to the wustite/magnetite interface ( $B_2$ ); (v) reaction with magnetite at layer surface forming wustite and gaseous products ( $A_2$ ); (vi) remaining reactants diffuse through the magnetite layer to the magnetite/hematite interface ( $B_1$ ); (vii) reaction with hematite core forming magnetite and a gaseous products ( $A_1$ ); (viii) The gaseous products diffuses outwards through the pores of the pellet. Since each step is a resistance to the total reduction of the pellet, the reduction pattern of a single pellet can be considered to follow a resistance network such as an electrical resistance circuit network. The solution of this resistance network yields the reaction flow rate of  $\dot{Y}_{j,i}$  of the gas species for the relative layers yields:

### From hematite to magnetite:

$$\begin{aligned} \dot{Y}_{h,i} &= ([A_3(A_2 + B_2 + B_3 + F) + (A_2 + B_2)(B_3 + F)](Y - Y_1^{eq}) \\ &\quad - [A_3(B_2 + B_3 + F) + B_2(B_3 + F)](Y - Y_2^{eq}) \\ &\quad - [A_2(B_3 + F)](Y - Y_3^{eq})) \frac{1}{W_{3,i}}, \end{aligned} \quad (20)$$

### From magnetite to wustite:

$$\begin{aligned} \dot{Y}_{m,i} &= ([A_1(A_2 + B_2) + A_3(B_3 + F)](Y - Y_2^{eq}) \\ &\quad - [B_2(A_3 + B_3 + F) + A_3(B_3 + F)](Y - Y_1^{eq}) \\ &\quad - [(A_1 + B_1)(B_3 + F)](Y - Y_3^{eq})) \frac{1}{W_{3,i}}, \end{aligned} \quad (21)$$

### From wustite to iron:

$$\begin{aligned} \dot{Y}_{w,i} &= ([A_1(A_2 + B_2 + B_3 + F) + A_2(B_2 + B_3 + F)] \\ &\quad (Y - Y_3^{eq}) - [A_2(B_3 + F)](Y - Y_1^{eq}) \\ &\quad - [(A_1 + B_1)(B_3 + F)](Y - Y_2^{eq})) \frac{1}{W_{3,i}} \end{aligned} \quad (22)$$

where the index  $i$  denotes the gas-species  $i$  (i.e. either CO or H<sub>2</sub>). Furthermore,  $A_j$  represents the relative chemical reaction resistance term,  $B_j$  the relative diffusivity resistance

term,  $j$  represents the layers hematite, magnetite and wustite and  $i$  the reducing gas species.  $F$  is the mass transfer resistance term, which is defined with  $1/k_f$ .  $Y$  is the bulk gas mole fraction and  $Y_j^{eq}$  the relative layer equilibrium mole fractions. The denominator  $W_{3,i}$  is expressed as

$$W_{3,i} = [(A_1 + B_1)(A_3(A_2 + B_2 + B_3 + F) + (A_2 + B_2)(B_3 + F)) + A_2(A_3(B_2 + B_3 + F) + B_2(B_3 + F))] \quad (23)$$

The chemical reaction resistance term  $A_{j,i}$  can be expressed as

$$A_{j,i} = \left[ \frac{1}{(1-f_j)^{\frac{2}{3}}} \frac{1}{k_j \left(1 - \frac{1}{Ke_j}\right)} \right]_i \quad (24)$$

in which  $j$  represents the reduction layer,  $i$  the reducing gas,  $k$  the reaction rate constant and  $f_j$  is the local fractional reduction of the relative layer that is calculated as

$$f_j = 1 - \left( \frac{r_j}{r_g} \right)^3. \quad (25)$$

The diffusivity resistance term  $B_{j,i}$  can be calculated for the relative iron oxide component as (Valipour *et al.*, 2006; Valipour, 2009)

$$B_{h,i} = \left[ \frac{(1-f_m)^{\frac{1}{3}} - (1-f_h)^{\frac{1}{3}}}{(1-f_m)^{\frac{1}{3}}(1-f_h)^{\frac{1}{3}}} \frac{r_g}{De_h} \right]_i, \quad (26)$$

$$B_{m,i} = \left[ \frac{(1-f_w)^{\frac{1}{3}} - (1-f_m)^{\frac{1}{3}}}{(1-f_w)^{\frac{1}{3}}(1-f_m)^{\frac{1}{3}}} \frac{r_g}{De_m} \right]_i, \quad (27)$$

$$B_{w,i} = \left[ \frac{1 - (1-f_w)^{\frac{1}{3}}}{(1-f_w)^{\frac{1}{3}}} \frac{r_g}{De_w} \right]_i, \quad (28)$$

in which  $De_j$  represents the diffusion coefficient of the relative layer.

With the use of the reaction flow rate  $\dot{Y}_{j,i}$  the relative mass flow rates between layers can be defined as

$$\frac{dm_i}{dt} = C_i M_i A_p \dot{Y}_{j,i}. \quad (29)$$

#### Mass and Heat Transfer Coefficient

The mass transfer coefficient  $k_f$  which is used in the determination of the mass transfer term can be calculated through the Sherwood number or the Nusselt number as

$$\begin{aligned} Sh &= \frac{k_f d}{D_e}, \\ Nu &= \frac{k_f}{k}, \end{aligned} \quad (30)$$

where  $d$  is the diameter of pellet,  $D_e$  the diffusion coefficient and  $k$  the thermal conductivity. A number of correlations for determining the Sherwood number exist in literature. Lee and Barrow (Lee and Barrow, 1968) proposed a model through investigating the boundary layer and wake regions around the sphere leading to a Sherwood number of

$$Sh_t = (0.51Re^{0.5} + 0.02235Re^{0.78})Sc^{0.33}, \quad (31)$$

where  $Sc$  stands for the Schmidt number and defined as  $\frac{\nu}{\rho D}$ . In more recent works from Valipour (Valipour, 2009) and

Nouri *et al.* (Nouri *et al.*, 2011) the Sherwood and Nusselt numbers are expressed as

$$\begin{aligned} Sh &= 2 + 0.6Re^{0.5}Sc^{0.33}, \\ Nu &= 2 + 0.6Re^{0.5}Pr^{0.33}. \end{aligned} \quad (32)$$

$Pr$  represents the Prandtl number and is expressed as the specific heat times the viscosity over thermal conductivity  $c\mu/k$ . However, since fluidized beds usually show very dense regions we use the correlation proposed by Gunn (1978) to compute the Nusselt number and consequently the heat transfer coefficient.

#### Diffusivity Coefficient

Diffusivity of a gaseous species depends on properties such as the pore size distribution, void fraction and tortuosity. For example, according to Tsay *et al.* (1976) a pore size of  $2\mu$  to  $5\mu$  the Knudsen diffusion has been found to be 10 times faster than molecular diffusion, therefore in their work the Knudsen diffusion has been neglected, since slowest process mostly determines the final reaction rate. Thus, the effective binary gas diffusion was calculated with

$$D_{eff} = D_{12} \frac{\epsilon}{\tau} \quad (33)$$

where  $\epsilon$  represents the dimensionless void fraction,  $\tau$  the tortuosity. (Valipour, 2009; Valipour *et al.*, 2006) has used the Fuller-Schettler-Giddings equation to determine the effective diffusivity as

$$D_{j,i} = \frac{10^{-7} T^{1.75}}{(P_t(\dot{v}_j^{1/3} + \dot{v}_i^{1/3}))^2} \left( \frac{1}{M_j} + \frac{1}{M_i} \right)^{0.5} \quad (34)$$

in which the  $\dot{v}$  is the diffusion volume of the relative species,  $M$  is the molecular weight,  $P_t$  the total flow pressure and  $T$  the temperature in Kelvin.

#### Reaction Rate Coefficient

For many reactions the rate expression can be expressed as a temperature-dependent term. It has been established that in these kinds of reactions, the reaction rate constant can be expressed with the Arrhenius' law (Levenspiel, 1999) as follows

$$k = k_0 \exp\left(\frac{-E_a}{RT}\right), \quad (35)$$

in which  $k_0$  represents the frequency factor or the pre-exponential factor,  $E_a$  the activation energy,  $R$  the universal gas constant and  $T$  the temperature. The values for the pre-exponential factor and the activation energy can be found through various works (Tsay *et al.*, 1976; Valipour, 2009).

## IMPLEMENTATION

Since the motion equation of the Lagrangian particles (equation (9)) does only account for collision implicitly by using equation (10) the total volume fraction of the tracer particles,  $\epsilon_{s,p} = \sum_{i=1}^{N_{sp}} n_i \pi d_{s,i}^3 / 6$  (compare with equation (5)) may exceed the maximum packing locally. This, in turn, may yield an unphysical accumulation of tracer particles in dense regions. Thus, we introduce an additional repulsive mechanism  $\mathbf{F}_k^{\text{pack}}$  (units  $\text{m s}^{-2}$ ), which prevents the Lagrangian tracer particles from forming dense aggregates exceeding the maximum packing fraction. Finally, the reduction model is evaluated at each parcel at each parcel time step. The resulting mass transfer and reaction heats have to be mapped to

the Eulerian grid to compute  $\mathcal{R}_i$  (equations (3) and (12)) and  $\mathcal{S}_q$  (equation (14)). For more details the reader is referred to equations (26) and (28) in our previous study (Schneiderbauer *et al.*, 2016b). Finally, it has to be noted that in the case where no tracer particle is in a specific numerical cell we apply a diffusive smoothing approach to the exchange fields locally (i.e. to the Sauter mean diameter; Pirker *et al.* (2011)).

For the numerical simulation we use the commercial finite volume CFD-solver FLUENT (version 16). For the discretization of all convective terms the QUICK (Quadratic Upwind Interpolation for Convection Kinematics) scheme is used. The derivatives appearing in the diffusion terms are computed by a least squares method and the pressure-velocity coupling is achieved by the phase coupled SIMPLE algorithm (Cokljat *et al.*, 2006). The trajectories of the Lagrangian tracer particles (equation (9)) is integrated after each fluid flow time step using a third-order Runge-Kutta method. Further it has to be noted that the gas velocity and the solid phase velocity in equation (9) are linearly interpolated to the particle positions by using a first order Taylor approximation. For fluidized bed simulations we employ a time step size of 0.001. More details on the implementation can be found in our previous studies (Schneiderbauer *et al.*, 2016a,b).

## RESULTS

To validate the presented reduction model, we investigate the direct reduction of hematite ore within a lab-scale fluidized bed with 68 mm diameter (Spreitzer, 2016). The small dimensions of the vessel allow to use very fine grid spacings (i.e.  $\approx 2$  mm), which resolve all relevant heterogeneous structures, and therefore no sub-grid corrections are required (Schneiderbauer *et al.*, 2013; Schneiderbauer and Pirker, 2014). The pressure in the fluidized bed was 140000 Pa and the superficial gas velocity  $0.25 \text{ m s}^{-1}$ . The detailed process conditions are given in tables 2, 3 and 4. According to table 3 we use four different types of tracer parcel representing the different size fractions. In total we found that 120000 tracer parcels are appropriate to gather sufficient statistics (Schneiderbauer *et al.*, 2016a,b).

**Table 2:** Experimental conditions for the different reduction steps. The concentrations of the reactants are given in volume percent.

	R1 (W→Fe)	R2 (M→W)	R3 (H→M)
H <sub>2</sub>	13.4%	15.9%	13.0%
H <sub>2</sub> O	3.4%	6.8%	6.8%
CO	37.0%	37.4%	30.3%
CO <sub>2</sub>	14.0%	27.4%	26.4%
N <sub>2</sub>	32.2%	12.4%	23.5%
T [°C]	720	750	480

**Table 3:** Particle size distribution of the iron ore.

$d_p$	fraction [vol. %]
0 – 0.063	0
0.063 – 0.125	15.4
0.125 – 0.25	33.2
0.25 – 0.5	28.6
0.5 – 1	22.8

Figure 1 shows snapshots of the solid volume fraction, the mass fraction of CO, the mass fraction of CO<sub>2</sub> and the frac-

**Table 4:** Parameters for DRI-model (Hanel *et al.*, 2015).

		H→M	M→W	W→Fe
H <sub>2</sub>	$k_0$ [m/s]	160	29	6
	$E_a$ [J]	68600	75000	65000
	$Ke$ [-]	$e^{\frac{-362.6}{T_s} + 10.334}$	$10^{\frac{-3577}{T_s} + 3.74}$	$10^{\frac{-827}{T_s} - 0.468}$
CO	$k_0$ [m/s]	437	45	17
	$E_a$ [J]	102000	86000	68000
	$Ke$ [-]	$e^{\frac{3968.37}{T_s} + 3.94}$	$10^{\frac{-1834}{T_s} + 2.17}$	$10^{\frac{914}{T_s} - 1.097}$

tional reduction of individual parcels during the conversion of hematite to magnetite. On the one hand, figure 1a unveils that the bed is operated in the bubbling regime to optimize the solid mixing, the gas-solid contact as well as the reaction heat removal. On the other hand, figures 1b – 1d clearly reveal the removal of oxygen from the hematite ore due to the conversion of CO to CO<sub>2</sub>, which increases the fraction reduction of the individual iron ore particles. In particular, the content of CO considerably decreases as the gas passes the particle bed while the content of CO<sub>2</sub> increases.

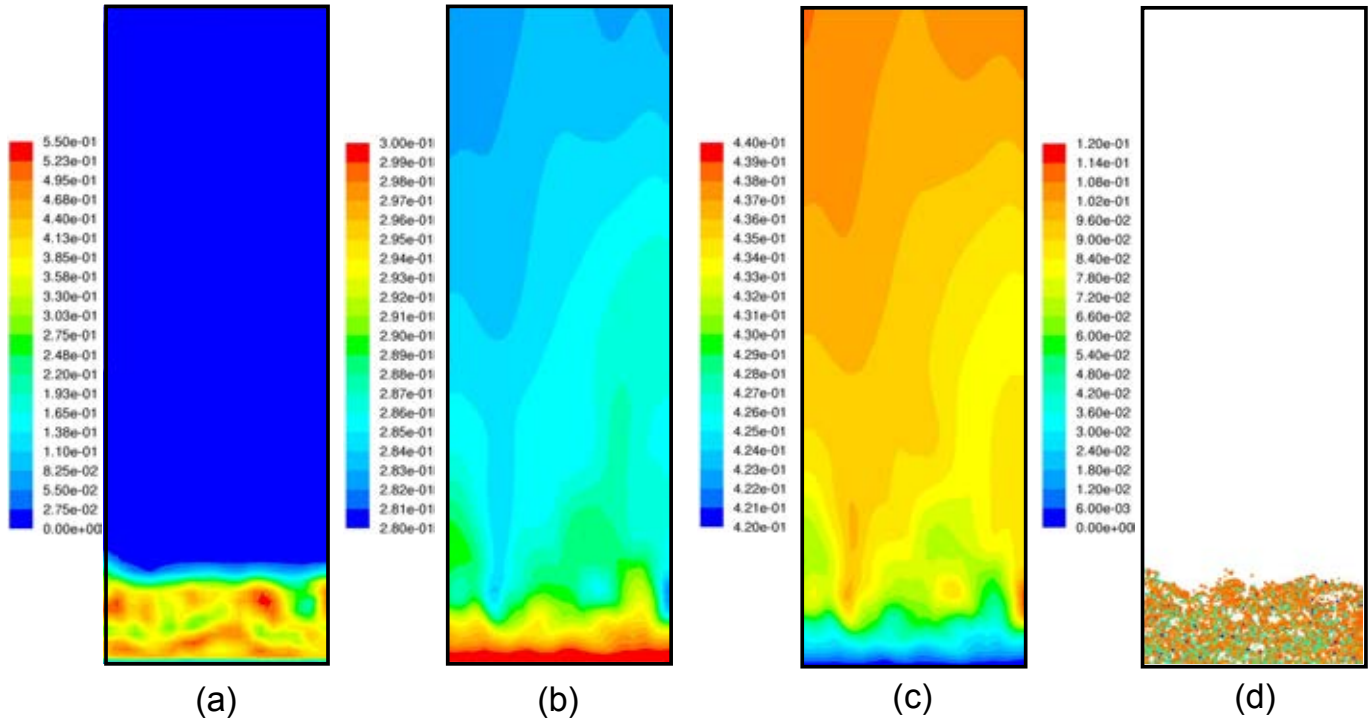
Figure 2 shows the cumulative distribution function of the fractional reduction. The figure indicates that after about 150 s approximately 50% of the hematite ore was converted to magnetite. In particular, the smallest particles are already converted after 150 s while the larger particles still contain hematite (figure 3). This is clear, since the larger particles contain much more hematite ore than compared to their surface area than the smaller particles.

Finally, figure 4 shows the fractional reduction as a function of time for the different reduction steps. Both, experiment and simulation unveil that the conversion of hematite to magnetite (R3) is the fastest reduction step (Hanel *et al.*, 2015). After approximately 500 s the fractional reduction approaches a plateau, where the fractional reduction is about 11.1%. Here, the total amount of hematite was already converted to magnetite. The subsequent conversion from magnetite to wustite is known to be the second fastest reduction step, which is also correctly predicted by the presented conversion model. Again, the fractional reduction approaches a plateau region, where the fraction reduction is about 33.3%, which is in fairly good agreement with the experiment. It has to be noted that we stopped the simulations after reaching the plateau regions of fractional correction during R3 and R2 and extrapolated the fractional correction in time in figure 4 till the next reduction step to reduce the computational demands. The final reduction step, where wustite is converted to metallic iron, unveils the slowest conversion rate. This is also indicated by the kinetic parameters given in table 4. Similar to the previous reduction steps, the present model is able to correctly predict the conversion of wustite to iron.

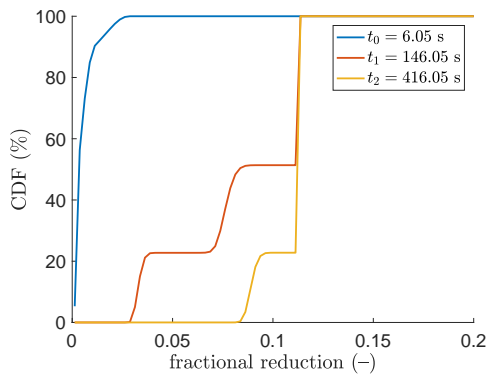
## CONCLUSION

We have presented the application of our previously published hybrid-TFM (Schneiderbauer *et al.*, 2015b; Schellander *et al.*, 2013; Pirker and Kahrmanovic, 2009; Schneiderbauer *et al.*, 2016a,b) to the conversion of iron ore to iron using fluidized bed technology. Such a modelling strategy enables the efficient numerical analysis of reactive poly-disperse gas-phase reactors without requiring computationally demanding multi-fluid models, which are coupled to population balance approaches.

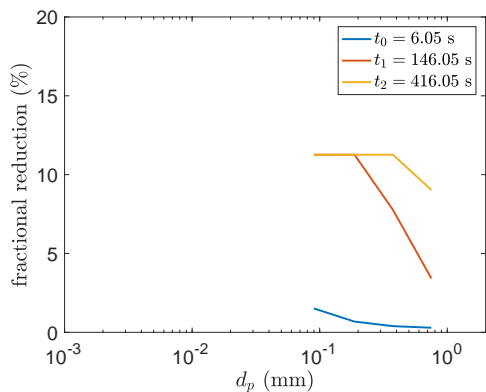
To conclude, the results clearly show that the reactive hybrid-TFM is able to picture the correct conversion rates within the fluidized bed. Nevertheless, the conversion model has to



**Figure 1:** Snapshots at  $t = 228$  s (i.e. within  $R_3$ ) of a) the solid volume fraction, b) the mass fraction of CO, c) the mass fraction of  $\text{CO}_2$  and d) the fractional reduction of individual parcels.

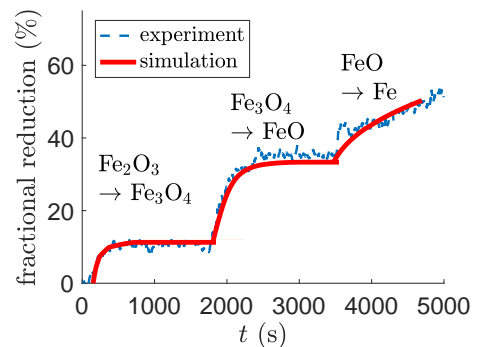


**Figure 2:** Snapshots of cumulative distribution of the fractional reduction during the conversion of hematite to magnetite.



**Figure 3:** Snapshots of the fractional reduction as a function of the particle diameter during the conversion of hematite to magnetite.

be verified further against more different gas compositions. I.e. future efforts will concentrate on the numerical analysis



**Figure 4:** ractional reduction as a function of time for the different reduction steps.

of different process conditions and their detailed evaluation against experimental data. Finally, large-scale applications should be investigated, where sub-grid corrections will be required to account for the unresolved small scales on the behaviour of the fluidized bed and the conversion rates (Schneiderbauer, 2017).

### ACKNOWLEDGEMENTS

The authors want to acknowledge the support of Dr. Christoph Klaus-Nietrost, who provided the c-code for the reduction model developed during his PhD work "Development of Conversion Models for Iron-Carriers and Additives within a Melter-Gasifier or Blast Furnace" (Institute for Energy Systems and Thermodynamics, TU Vienna, 2016). This work was funded by the Christian-Doppler Research Association, the Austrian Federal Ministry of Economy, Family and Youth, and the Austrian National Foundation for Research, Technology and Development. The author also wants to acknowledge the financial support from the K1MET center for metallurgical research in Austria ([www.k1-met.com](http://www.k1-met.com)).



## REFERENCES

- AGRAWAL, K., LOEZOS, P.N., SYAMLAL, M. and SUNDARESAN, S. (2001). "The role of meso-scale structures in rapid gas-solid flows". *Journal of Fluid Mechanics*, **445**, 151–185.
- ANSYS (2011). *ANSYS FLUENT Theory Guide*, vol. 15317. ANSYS, Inc., Canonsburg, PA.
- BEETSTRA, R., Van der Hoef, M.A. and KUIPERS, J.A.M. (2007). "Drag Force of Intermediate Reynolds Number Flow Past Mono- and Bidisperse Arrays of Spheres". *AIChE Journal*, **53**(2), 489–501.
- COKLIJAT, D., SLACK, M., VASQUEZ, S.A., BAKKER, A. and MONTANTE, G. (2006). "Reynolds-Stress Model for Eulerian multiphase". *Progress in Computational Fluid Dynamics, An International Journal*, **6**(1/2/3), 168.
- FU, D., ZHOU, C.Q. and CHEN, Y. (2014). "Numerical Methods for Simulating the Reduction of Iron Ore in Blast Furnace Shaft". *Journal of Thermal Science and Engineering Applications*, **6**(2), 021014.
- GONIVA, C., KLOSS, C., DEEN, N.G., KUIPERS, J.A.M. and PIRKER, S. (2012). "Influence of rolling friction on single spout fluidized bed simulation". *Particuology*, **10**(5), 582–591.
- GUNN, D.J. (1978). "Transfer of Heat or Mass to Particles in Fixed and Fluidized Bed". *International Journal of Heat Mass Transfer*, **21**, 467–476.
- HABERMANN, A., WINTER, F., HOFBAUER, H., ZIRNGAST, J. and SCHENK, J.L. (2000). "An Experimental Study on the Kinetics of Fluidized Bed Iron Ore Reduction". *ISIJ International*, **40**(10), 935–942.
- HANEL, M.B., SCHENK, J.F., MALI, H., HAUZENBERGER, F., THALER, C. and STOCKER, H. (2015). "Characterization of Ferrous Burden Material for Use in Ironmaking Technologies". *BHM Berg- und Hüttenmännische Monatshefte*, **160**(7), 316–319.
- HRENYA, C.M. and SINCLAIR, J.L. (1997). "Effects of particle-phase turbulence in gas-solid flows". *AIChE Journal*, **43**(4), 853–869.
- IDDIR, H. and ARASTOPOUR, H. (2005). "Modeling of multitype particle flow using the kinetic theory approach". *AIChE Journal*, **51**(6), 1620–1632.
- KINACI, M.E., LICHTENEGGER, T. and SCHNEIDERBAUER, S. (2017). "Modelling of Chemical Reactions in Metallurgical Processes". J.E. Olsen (ed.), *Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries (CFD 2017)*. SINTEF, Trondheim, Norway, Trondheim, Norway.
- LEE, K. and BARROW, H. (1968). "Transport processes in flow around a sphere with particular reference to the transfer of mass". *International Journal of Heat and Mass Transfer*, **11**(6), 1013–1026.
- LEVENSPIEL, O. (1999). *Chemical Reaction Engineering*.
- LUN, C.K.K., SAVAGE, S.B., JEFFREY, D.J. and CHEPURNIY, N. (1984). "Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flowfield". *Journal of Fluid Mechanics*, **140**, 223–256.
- NATSUI, S., KIKUCHI, T. and SUZUKI, R.O. (2014). "Numerical Analysis of Carbon Monoxide-Hydrogen Gas Reduction of Iron Ore in a Packed Bed by an Euler-Lagrange Approach". *Metallurgical and Materials Transactions B*, **45**(6), 2395–2413.
- NOURI, S.M.M., Ale Ebrahim, H. and JAMSHIDI, E. (2011). "Simulation of direct reduction reactor by the grain model". *Chemical Engineering Journal*, **166**(2), 704–709.
- PIRKER, S. and KAHRIMANOVIC, D. (2009). "Modelling Mass Loading Effects in Industrial Cyclones by a Combined Eulerian-Lagrangian Approach". *Acta Mechanica*, **204**(2), 203–216.
- PIRKER, S., KAHRIMANOVIC, D., KLOSS, C., POPOFF, B. and BRAUN, M. (2010). "Simulating coarse particle conveying by a set of Eulerian, Lagrangian and hybrid particle models". *Powder Technology*, **204**(2-3), 203–213.
- PIRKER, S., KAHRIMANOVIC, D. and GONIVA, C. (2011). "Improving the applicability of discrete phase simulations by smoothing their exchange fields". *Applied Mathematical Modelling*, **35**(5), 2479–2488.
- PLAUL, F.J., BÖHM, C. and SCHENK, J.L. (2009). "Fluidized-bed technology for the production of iron products for steelmaking". *Journal of the Southern African Institute of Mining and Metallurgy*, **109**(2), 121–128.
- Primetals Technologies Austria GmbH and POSCO E&C (2015). "The finex® process – economical and environmentally safe ironmaking". <http://www.primetals.com/en/technologies/ironmaking/finex%C2%AE/Lists/FurtherInformation/The%20Finex%20process.pdf>. Accessed: 2017-02-28.
- RADL, S. and SUNDARESAN, S. (2014). "A drag model for filtered Euler-Lagrange simulations of clustered gas-particle suspensions". *Chemical Engineering Science*, **117**, 416–425.
- SHELLANDER, D., SCHNEIDERBAUER, S. and PIRKER, S. (2013). "Numerical study of dilute and dense poly-dispersed gas-solid two-phase flows using an Eulerian and Lagrangian hybrid model". *Chemical Engineering Science*, **95**, 107–118.
- SCHENK, J.L. (2011). "Recent status of fluidized bed technologies for producing iron input materials for steelmaking". *Particuology*, **9**(1), 14–23.
- SCHNEIDERBAUER, S. (2017). "A spatially-averaged two-fluid model for dense large-scale gas-solid flows". *AIChE Journal*.
- SCHNEIDERBAUER, S. and PIRKER, S. (2014). "Filtered and heterogeneity based sub-grid modifications for gas-solid drag and solids stresses in bubbling fluidized beds". *AIChE Journal*, **60**(3), 839–854.
- SCHNEIDERBAUER, S., AIGNER, A. and PIRKER, S. (2012). "A comprehensive frictional-kinetic model for gas-particle flows: analysis of fluidized and moving bed regimes". *Chemical Engineering Science*, **80**, 279–292.
- SCHNEIDERBAUER, S., PUTTINGER, S. and PIRKER, S. (2013). "Comparative Analysis of Subgrid Drag Modifications for Dense Gas-Particle Flows in Bubbling Fluidized Beds". *AIChE Journal*, **59**(11), 4077–4099.
- SCHNEIDERBAUER, S., PUTTINGER, S., PIRKER, S., AGUAYO, P. and KANELLOPOULOS, V. (2015a). "CFD Modeling and Simulation of Industrial Scale Olefin Polymerization Fluidized Bed Reactors". *Chemical Engineering Journal*, **264**, 99–112.
- SCHNEIDERBAUER, S., PUTTINGER, S. and PIRKER, S. (2015b). "Numerical study of a bi-disperse gas-solid fluidized bed using an Eulerian and Lagrangian hybrid model". *Procedia Engineering*, **102**, 1539–1545.
- SCHNEIDERBAUER, S., HAIDER, M.F., HAUZENBERGER, F. and PIRKER, S. (2016a). "A Lagrangian-Eulerian Hybrid Model for the Simulation of Industrial-scale

Gas-solid Cyclones”. *Powder Technology*, **304**, 229—240.

SCHNEIDERBAUER, S., PIRKER, S., PUTTINGER, S., AGUAYO, P., TOULOUPIDIS, V. and Martínez Joaristi, A. (2016b). “A Lagrangian-Eulerian Hybrid Model for the Simulation of Poly-disperse Fluidized Beds: Application to Industrial-scale Olefin Polymerization”. *Powder Technology* (*in press*).

SPREITZER, D. (2016). *Optimierung der Prozessparameter für die Reduktion von Feineisenerzen mittels Wirbelschichtverfahren*. Master thesis, Montanuniversität Leoben.

SYAMLAL, M., ROGERS, W. and O’BRIEN, T.J. (1993). “MFIx documentation theory guide, Technical note”. Tech. Rep. December, U.S. Department of Energy, Office of Fossil Energy, Morgantown, West Virginia.

TSAY, Q.T., RAY, W.H. and SZEKLEY, J. (1976). “The modeling of hematite reduction with hydrogen plus carbon monoxide mixture”. *AIChE J*, **22(6)**, 1064–1076.

VALIPOUR, M.S. (2009). “Mathematical Modeling of a Non-Catalytic Gas-Solid Reaction : Hematite Pellet Reduction with Syngas”. *Transactions C: Chemistry and Chemical Engineering*, **16(2)**, 108–124.

VALIPOUR, M.S., Motamed Hashemi, M.Y. and SA-BOOHI, Y. (2006). “Mathematical modeling of the reaction in an iron ore pellet using a mixture of hydrogen, water vapor, carbon monoxide and carbon dioxide: an isothermal study”. *Advanced Powder Technology*, **17(3)**, 277–295.