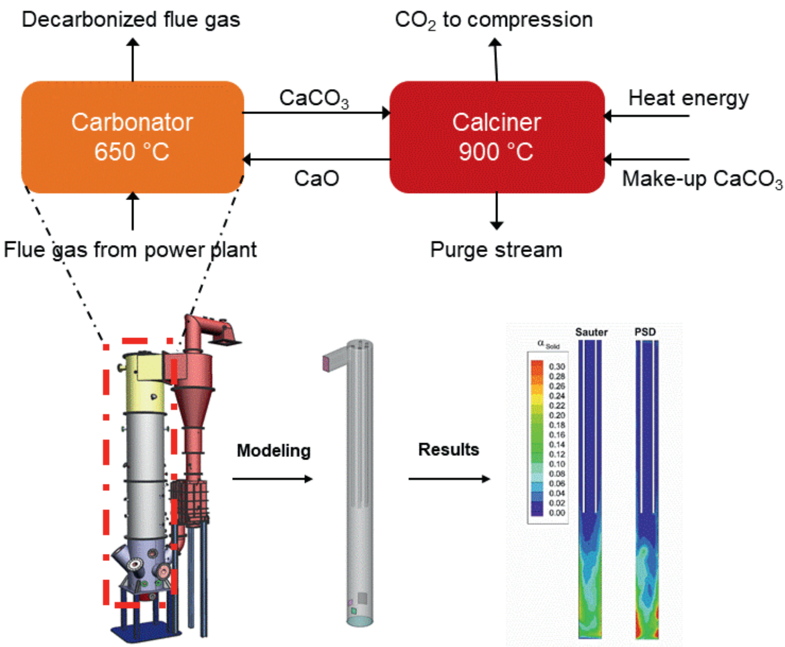
Development of a 3D Model for the Numerical Simulation of a Reactive Fluidized Bed Carbonator

Alexander Stroh



Development of a 3D Model for the Numerical Simulation of a Reactive Fluidized Bed Carbonator

Vom Fachbereich Maschinenbau
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zur
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vorgelegt von

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Preface

The present Ph.D. thesis *Development of a 3D Model for the Numerical Simulation of a Reactive Fluidized Bed Carbonator* is the result of my time as a doctoral candidate at the Department of Energy Systems and Technology at the Technische Universität Darmstadt. I would like to express my gratitude to all those who gave me the possibility to complete this thesis.

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Table of Contents

Nomenclature

Latin symbols

A	vessel cross–section area	$[m^2]$
a	translational acceleration	$[m/s^2]$
B	magnetic flux density	[N/A m]
C	molar gas concentration, drag coefficient	$[mol/m^3]$, [−]
D	surface diffusion coefficient, volume diffusion coefficient	$[m^2/s]$, $[m^3/s]$
D	thermophoretic coefficient	[−]
d	diameter, deformation tensor	[−]
E	electric field intensity, energy	[N/A s] , [J]
ER	expansion ratio	[−]
e	east	[−]
F	force	[N]
FI	fluidization index	[−]
FR	fluctuation ratio	[−]
f	volume fraction in micro-scale dense-phase, function	[−]
g	standard gravity	$[m/s^2]$
H	magnetic field strength, heterogeneity index	[A/m], [−]
h	enthalpy, height	[kJ/kg], [m]
$\dot{h}$	heat flux	$[W/m^2]$
$\mathbf{I}$	unit matrix	[−]
I	moment of inertia	$[kg\ m^2]$
J	matrix for computational method	[−]
k	stiffness coefficient, reaction rate constant	[N/m], [1/s]
l	length	[m]
M	molar mass, statistic moment	[kg/kmol], [−]
m	mass, mass fraction of gas species	[kg], [−]
$\dot{m}$	mass flow rate	[kg/s]
N	number of particles	[−]
n	normal vector	[−]
p	pressure	$[N/m^2]$
Q	cumulative distribution function	[−]
q	charge, probability distribution function	[A s], [−]
R	volume ratio of parcel to particle	[m], [−]
r	radius, position vector	[m], [m]
S	source term, available reaction surface area	[different], $[m^2]$
T	temperature, computing time	[N m], [K], [s]

T	stress tensor for Newtonian fluids	[N/m^2]
t	time	[s]
u	translational velocity, fluidization velocity, internal energy	[m/s], [kJ/kg]
V	volume	[m^3]
v	velocity magnitude	[m/s]
$\dot{V}$	volume flow rate	[m^3/s]
W	inventory, potential energy	[kg], [J]
w	weight factor, west	[−]
X	conversion degree of CaO to $CaCO_3$	[−]
Y	gas species	[−]
x, y, z	cartesian coordinates, distance vector	[m]

Greek symbols

α	heat transfer coefficient, collision angle, volume fraction	[W/K m^2], [rad], [−]
β	momentum exchange coefficient, restitution coefficient	[kg/s m^3], [−]
γ	damping coefficient	[kg/s]
δ	penetration depth	[m]
ε	voidage, dissipation rate	[−], [m^2/s^3]
Θ	blending factor	[−]
η	restitution coefficient, CO_2 capture efficiency	[−], [−]
λ	thermal conductivity, bulk viscosity	[W/K m], [kg/m s]
λ	free path length of the fluid, parcel to particle diameter ratio	[m], [−]
μ	dynamic viscosity, friction coefficient, relative permeability	[kg/m s], [−], [−]
μ_r	rolling friction coefficient	[m]
ρ	density	[kg/m^3]
τ	viscous stress, particle relaxation time	[N/m^2], [s]
ν	kinematic fluid viscosity	[m^2/s]
ϕ	physical value, sphericity of the solid	[different], [−]
Ω	relative angular velocity particle-fluid	[rad/s]
ψ	stitching function for smoother transition	[−]
ω	angular velocity	[rad/s]

Constants

R	universal gas constant	[N m/kmol K]
μ_0	magnetic field constant $4\pi \cdot 10^{-7}$	[N/A^2]
π	mathematical constant, 3.14159265359	[−]

Dimensionless numbers

Ar	Archimedes number
Kn	Knudsen number
Pe	Peclet number
Pr	Prandtl number
Re	Reynolds number
St	Stokes number

Subscripts and indices

b	bed

bub	bubble
buo	buoyancy
c	velocity at maximum standard deviation of pressure fluctuations
char	characteristic
cir	circulating
cl	cluster
coll	collision
con	contact
crit	critical
d	drag
ER	expansion ratio
e	east, turnover time of large eddies
el	electrical
en	envelope density
eq	equilibrium
equ	equivalent
FR	fluctuation ratio
f	fluid
g	gas
gra	gravitation
hor	horizontal
hyd	hydrodynamic
i	component, notation, particle index
j	component, notation, particle index
k	characteristic velocity for fluidization regime
max	maximum
min	minimum
n	normal
nb	neighbor cells
op	operating
p	particle
parcel	numerical particle
pot	potential energy
r	rolling, defining type of CDF/PDF function
relax	relaxation
slip	slip velocity between gas and particle
st	suspension & transport of particles
stat	static
T	thermophoretic
t	tangential, terminal, turbulence
tr	transport velocity
V	volume
ver	vertical
ves	vessel

vm	virtual mass
w	west
ω	angular variable

Chemical symbols

CO_2	carbon dioxide
Ca	calcium
CaO	calcium oxide
$CaCO_3$	calcium carbonate
$CaSO_4$	calcium sulphate
$Ca(OH)_2$	calcium hydroxide
H_2	hydrogen
H_2O	water
HBr	hydrogen bromide
NO_x	nitrogen oxides
O_2	oxygen
OH^-	hydrogen oxide
SO_x	sulphur monoxide/dioxide/trioxide
ΔH_0	standard enthalpy of reaction

Abbreviations

AMG	algebraic multigrid
IPCC	intergovernmental panel on climate change
CPFD	commercial CFD software
BET	Brunauer-Emmett–Teller method
CaL	carbonate looping process
CCS	carbon capture and sequestration
CDF	cumulative distribution function
CERTH	centre of research and technology applications
CFB	circulating fluidized bed
CFD	computational fluid dynamics
CPERI	chemical process & energy resources institute
CPU	central processing unit
DEM	discrete element method
DDPM	dense discrete particle model
DNS	direct numerical simulation
EMMS	energy minimization multiscale method
EST	energy systems and technology department
FI	fluidization index
FSM	fractional step method
GDP	gross domestic product
GPU	graphical processing unit
HPC	high performance computer
HRIC	high resolution interface capturing
ILU	incomplete lower upper decomposition
KTGF	kinetic theory of granular fluids

LES	large eddy simulation
MP-PIC	multiphase particle-in-cell
MUSCL	monotonic upwind scheme for conservation laws
NITA	non-iterative time advancement scheme
OECD	organisation for economic cooperation and development
PCM	particle centre method
PDF	probability distribution function
PSD	particle size distribution
PIC	particle–in–cell method
PISO	pressure–implicit with splitting of operators
QUICK	quadratic upwind interpolation for convective kinematic
RANS	Reynolds averaged Navier–Stokes method
RC	restitution coefficient
RMS	root mean square
RS	Reynolds stress
RSM	Reynolds stress model
SSP	same size parcel method
SSW	same statistic weight method
TFM	two-fluid model
TGA	thermogravimetric analysis
TUD	Technische Universität Darmstadt
SEM	scanning electron microscope
SIMPLE	semi–implicit method for pressure–linked equations
SIMPLEC	semi–implicit method for pressure–linked equation consisten

Abstract

The global warming has reached tremendous dimensions in form of water scarcity and long droughts periods [1]. Not only in the southern hemisphere, but also in Germany the average temperatures raised since year 2000. There are several possibilities to mitigate the climate change and the effects for humans on the world. Firstly, by reduction of energy consumption, food waste and mass-market consumables which in turn require also energy for their production. Another possibility is the application of Carbon Capture and Storage (CCS) technologies which has been scientifically researched for several years at the institute of Energy Systems and Technology in Darmstadt. One of the most promising technologies is the carbonate looping (CaL) process, due to the small efficiency penalties in comparison to other CCS technologies. The CaL process at EST consists of two interconnected circulating fluidized bed reactors in 1-MW scale, carbonator and calciner respectively [2]. The operation of such fluidized bed reactors in combustion and gasification applications has been already industrialized to large scale however with little understanding of the reactor gas-solid hydrodynamics. The process operation and sorbent behaviour in the context of CaL process is even in a younger stage, aiming to up-scale the process to 20 MW size. There are only limited experimental research works for large or semi-industrial test facilities available due to operational challenges in terms of complexity and costly measurement apparatus for obtaining the flow characteristics. The difficulties for the research arise in the complex hydrodynamics in fluidized beds and the accurate prediction of thermoreactive gas-solid mixtures.

Nowadays, in the era of increasing computational hardware performance, numerical simulations that are often referred as computational fluid dynamics (CFD) tools, have gained more attention. CFD tools allow to reduce the number of experiments in order to optimize a process through shortening the planning and construction time. Furthermore, the CFD results allow the evaluation of microscopic and macroscopic flow field variables that are difficult to measure in experiments. For these reasons, CFD tools are gaining fundamental importance to understand the phenomena taking place in fluidized bed applications. There are two important methods for modelling gas-solid flows, namely the Euler-Euler and Euler-Lagrange models. While for the first approach numerous works of circulating fluidized bed (CFB) applications exist, the second approach is rather rarely used for the simulation of large scale CFB units due to the high computational demand. This gives rise to this work, which is focused on the development of a 3D numerical model for the carbonator. In the applied Euler-Lagrange approach, the particle-particle and particle-wall collisions are computed by deterministic algorithms by using the soft-sphere approach. In this approach two colliding partners can overlap each other, leading to a penetration depth from which the collision force value during collision is evaluated. A special emphasis lies in defining appropriate numerical settings to simulate CFB systems at certain accuracy within a reasonable computational time. The gas-solid interactions are mainly calculated by so-called drag models that are either based on theoretical or semi-empirical models.

The objective of this work is to develop and evaluate a numerical model using the coupled Euler-Lagrange method with deterministic particle tracking scheme (CFD-DEM) for the simulation of the carbonator reactor in the CaL process. The particle-particle, particle-wall and particle-gas interactions are modelled by a reduced tracking scheme. The numerical tracking scheme is simplified in order to reduce the computational time that otherwise would result from the trajectory computation of several billions of particles. The modelling approach applied here is known as coarse graining method. In this approach so-called representative particles, called parcels, are tracked in the domain. The parcel is a representative numerical particle with the same material properties such as density and inner porosity as the real particles of the gas-solid system. The number of tracked particles is reduced to a reasonable value below 1 million, which allowed to carry out simulations of the carbonator within a reasonable time. The model development is carried out in three steps. In the first step, simulations of a lab-scale spouted fluidized bed reactor are performed in order to understand the effects of the restitution coefficient and tangential friction parameters during the collision evaluation for two different fluidization velocities using the coupled CFD-DEM approach. The advantage of the small-scale model gives the opportunity to evaluate the friction parameters and restitution coefficient influence using high-speed camera recordings and derive the optimal values for the larger scale simulations. In the second step, the coupled CFD-DEM model is applied to the simulation of the cold flow circulating fluidized bed reactor that is a down-scaled reactor model of the carbonator reactor of the 1 MW_{th} CaL plant. The cold flow 3-D circulating fluidized bed reactor was simulated at three fluidization velocities, using sand and glass beads as inventories. The drag models by Gidaspow and Energy Minimization Multiscale theory were applied to a polydisperse numerical simulation and the results were validated by experimental capacitance probe measurements of particle velocities and particle concentration. Furthermore, the reactor solid outflux, the total pressure drop over the reactor, and relative static pressure in several reactor heights were compared with experimental measurements. In the last step, the 1 MW carbonator was simulated using appropriate numerical settings based on the previous gained modeling experience. The numerical results were compared from long-term CaL tests using hard coal as fuel in the calciner. Numerically, the influence between the mean Sauter diameter and a particle size distributions from different extraction locations of the carbonator, for the numerical representation of the bed material, is investigated. The results accuracy of a PSD particle simulation is higher than in a case of monodisperse particle simulation. The numerical results of an implemented thermoreactive model for the carbonation reaction are compared with gas concentrations measurements downstream the cyclone and a complementary discussion using thermogravimetric analysis results of bed material from long term test campaigns is carried out. The good agreement between numerical and experimental results, as well as the computational efficiency of the 3D carbonator model in 1-MW scale, suggests the employment of the developed model for scale-up of the CaL process and other fluidized bed applications.