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Numerical investigation and comparison of coarse grain CFD – DEM and TFM in the case of a 1 MW_{th} fluidized bed carbonator simulation

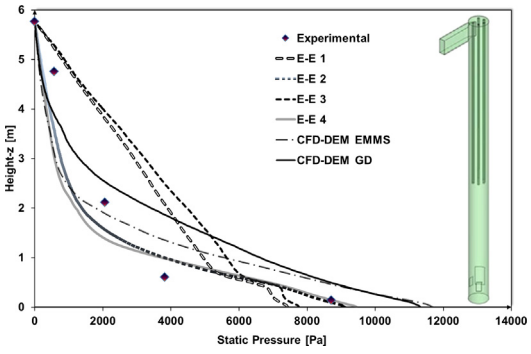
A. Nikolopoulos [a,*], A. Stroh [b,*], M. Zeneli [a,c], F. Alobaid [b], N. Nikolopoulos [a], J. Ströhle [b], S. Karellas [c], B. Epple [b], P. Grammelis [a]

[a] Centre of Research and Technology Applications Chemical Process & Energy Resources Institute (CERTH/CPERI), Thessaloniki, Greece
[b] Technische Universität Darmstadt, Institute for Energy Systems and Technology, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany
[c] Laboratory of Steam Boilers and Thermal Plants, National Technical University of Athens, 9 Heroon Polytechniou Street, 15780 Zografou, Greece

HIGHLIGHTS

- CFD-DEM and Euler-Euler comparison for CFB simulation.
- EMMS drag model increases the accuracy of both models.
- Cell length to parcel diameter ratio of less than 3 reproduced results of adequate accuracy.
- Parcel diameter to particle diameter of below 60 reproduced good results for the pressure profile.

GRAPHICAL ABSTRACT



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ABSTRACT

This work focuses on a comparison between the Euler-Euler Two Fluid Model (TFM) approach and the coupled coarse grain discrete element CFD-DEM numerical model for the simulation of a 1 MW_{th} CFB carbonator reactor located at TU Darmstadt (TUD). The effect of the drag force formulation and its associated application in the numerical model for both approaches in terms of their numerical accuracy, compared to experimental data is investigated, by implementing either the conventional Gidaspow model or the advanced EMMS one. Moreover, for the coarse grain CFD – DEM model, the range of values for important numerical parameters as the particle per parcel and cell to parcel size ratios are investigated to shed light on the necessary resolution such a model should have in order to reproduce valid and not parameter dependent numerical results. An adequate cell length to parcel diameter ratio is found to be around 2.6 while as concerns the parcel to particle diameter ratio a value around 58.5 proved to be sufficient, at least for the range of parameters investigated in this paper (size of riser, flow rates and particles average diameter). The EMMS model improved the accuracy of results derived by the coarse grain CFD – DEM model, while further research on the appropriate drag models for the coarse grain CFD – DEM is a *sine qua non* for its successful implementation in similar studies. For instance it is of interest to answer whether the individual particles slip velocity instead of the particles cell averaged slip, should be used for the calculation of the momentum interexchange coefficient (β) as well as the treatment of different particle diameters in the EMMS equation scheme.

* Corresponding authors.
E-mail address: a.nikolopoulos@certh.gr (A. Nikolopoulos).

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Nomenclature

α	parameter for the Gaussian distribution [–]
β	inter-phase momentum exchange coefficient [kg/(m^3 s)]
γ	damping coefficient [–]
δ	parcel overlap [m]
η	coefficient of restitution for the dashpot term
Δx	cell characteristic lenght [m]
ε_q	volume fraction of phase q [–]
ϑ	drag related term [kg m^{-2}]
μ	friction coefficient
μ_g	gas viscosity [kg/(m s)]
ξ	particle slip velocity minus the cell slip velocity [m s^{-1}]
ρ_q	density of phase q [kg/m^3]
φ	specularity coefficient [–]
A_N	forces ratio [–]
C_r	cell characteristic length to parcel diameter ratio [–]
D_{cell}	equivalent cell size [m]
d_p	particle diameter [m]
$F_{con,i}$	collision force [N]
f_{loss}	loss factor (DEM model parameter) [–]
F_x	force [N m^{-3}]
g	gravitational acceleration [m s^{-2}]
H_d	heterogeneity index [–]
k	spring stiffness constant [N m^{-1}]
l_r	cell characteristic length to particle diameter ratio [–]
m_{ij}	reduced mass (DEM model parameter) [kg]
N	number of particles/parcels in a cell [#]
P	pressure [Pa]
Pa_r	parcel to particle diameter ratio [–]
t	time [s]
t_{coll}	collision time scale (DEM model parameter) [s]
$\bar{\bar{\tau}}_q$	viscous stress tensor of phase q [Pa]
U_t	terminal velocity of a single particle [m s^{-1}]
u_q	velocity of phase q [m s^{-1}]
$v_{i,j}$	relative velocity between parcels i, j
V	gas parcel slip velocity [m s^{-1}]
w	weighting factor for the kernel [–]
x_{node}	position vector of cell verticies [m]
x_p	position vector of particles[m]

Sub- and super scripts

ι	x, y, z direction
$\|\|\|$	magnitude of a vector
c	cell
cn	cell node
coll	collision
con	contact
E	in an Eulerian fashion
g	gas
i, j	parcel indices
L	in a Lagrangian fashion
mf	minimum fluidization
n	normal
p	particle
s	solid phase
t	tangential
x′	deviation of x

1. Introduction

In the early Fluidized Bed (FB) development stage, lab-scale experiments lead to empirical approaches for calculating the range of values for various operating fluidization regimes and/or technical aspects e.g. minimum fluidization velocity, bubble formation, particle attrition and axial solid mass fraction distribution depending on the fluid-solid properties (Adánez and Abanades, 1991; Samuelsberg and Hjertager, 1996; Mathiesen et al., 2000; Min et al., 2010). Such lab-scale experiments of fluidized bed reactors provided the basis for commercial scale reactor design. However, in the last decade due to increasing development of the available computational resources, numerical models and simulations gained particular importance as a supporting tool for the prediction of gas-solid flow characteristics for the case of fluidized beds, contributing to the examination of design parametric modifications by complementing experimental data. Nonetheless, there is still a need to further investigate the capacity of available computational fluid dynamics (CFD) tools and examine the current range of validity of the currently available model approaches against experimental measurements derived from experimental campaigns conducted for the purposes of fluidized beds, either operating as combustors, catalytic crackers or even CO_2 absorbers. The ultimate goal is to provide highly accurate and sophisticated models with a reasonable and affordable computational cost.

This paper tries to shed light about the available modeling approaches by comparing the Euler – Euler approach and the recently developed coarse grain CFD-DEM, for the single case of a fluidized bed carbonator used as one of the two interconnected reactors in the process of Calcium-Looping. The comparison of the available model approaches is based on the availability of experimental measurements of a 1 MW_{th} CFB carbonator located at the premises of Technical University Darmstadt (TUD). The CFD-DEM coarse grain approach is in depth investigated in terms of drag calculations, grid and grain/parcel size resolution as well as parcel velocity sub-grid distribution.

1.1. Modeling approaches

The two – phase flow within FBs is rather complicated and the corresponding CFD modeling is not trivial. A lot of different approaches exist on how to fundamentally simulate each phase. Trying to categorize them, a first approach is the direct numerical simulation of particles flow characteristics. Such an approach, being in position to resolve the flow around the particles with body fitted numerical grids, necessitates for high resolution models as presented by (Cho et al., 2005). These models can handle hundreds or even thousands of particles but for the case of real practical applications (especially for the case of industrial scale units) with the presence of million or even billion particles they are not today easily affordable owing to lack of sufficient CPU resources. As (Tsuji et al., 1993) predicted in the past it is impossible even for modern super-computers to simultaneously solve micro and macro scale phenomena; this drove the majority of the authors to use models that are based on locally averaged quantities (Anderson and Jackson, 1967). However, during the recent years GPU computing seems promising for feasible simulations of engineering applications. Lately, a quasi-real-time simulation of an industrial rotating drum, by means of 270 GPUs, has been achieved with 10 million centimeter-size particles giving hopes for future simulations (Xu et al., 2011).

Generally, one may distinguish between two modeling approaches for conventional simulations of gas-particle flows, i.e. the Euler-Euler method, also known as two-fluid model, and the coupled Euler-Lagrange method. Following the comprehensive review work of (Sundaresan, 2011) and trying to classify such models, the following rough categorization is proposed, Fig. 1 and Table 1.