NUMERICAL SIMULATION OF FLUIDIZATION FOR APPLICATION IN OXYFUEL COMBUSTION

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Abstract. This paper is concerned with the simulation of multiphase flow hydrodynamics in an experimental oxyfuel fluidized bed combustor designed for biomass fuels. The aim is to perform cross-validation between several models and solvers that differ in the description of some phenomena in question. We focus on the influence of turbulence modeling, inter-phase drag force models, the presence of biomass in the mixture. Also the possibility to simplify the full 3D description to a quasi-1D model is tested. However, the results indicate that such simplification is not suitable for chaotic phenomena in considered scenarios. The models were developed using ANSYS Fluent and OpenFOAM CFD software packages as well as our in-house CFD code CFBSim. The quantities relevant for comparison (the densities of the dispersed solid phases and the phase velocities) are presented in the form of cross-section averaged vertical profiles.

1. Introduction. Combustion of fossil and renewable fuels is a significant contributor to energy production worldwide. In order to reduce carbon dioxide emissions, promising technologies of carbon capture and storage [10] are under development. For efficient separation of CO₂ from the flue gases, oxyfuel combustion [14] has been proposed. Large concentrations of CO₂ in the flue gas are achieved by using pure oxygen as oxidizer instead of air and by flue gas recirculation. By employing oxyfuel technology in combination with fluidized bed boilers [2], fuels with a large fraction of biomass can successfully be used, leading to a negative carbon footprint of such energy production method.

The main aim of our team is to develop a complex mathematical model and simulation software useful in the investigation, optimization, and control of the operation of oxyfuel fluidized bed boilers. At the moment, we mainly consider laboratory scale devices, and we focus on their central component - the combustion chamber.

Our modeling technique is based on the multi-phase continuum dynamics - see, e.g. [5, 12], involving the conservation laws of the corresponding quantities, the constitutive laws, and empirical relations (see, e.g., [2, 7, 3]).

In view of the complexity of the resulting models, it is necessary to introduce simplifications (such as quasi-1D vs. full 3D flow description). The effect of

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simplifications and the choice of the individual sub-models needs to be verified and validated.

In this paper, we compare several models of fluidization (multiphase flow without combustion) and investigate the influence of different approaches to modeling turbulence, compressibility, inter-phase drag forces, etc. The models were developed using established CFD software packages ANSYS Fluent and OpenFOAM as well as our in-house CFD code CFBSim. The target system to be modeled is an experimental fluidized bed combustor \cite{11}. The model parameters are set to resemble hydrodynamic conditions during oxyfuel combustion of biomass.

2. Mathematical model. For the scope of this paper, we consider a simplified isothermal multiphase flow regimes without the combustion and chemical reactions. The hydrodynamics is studied in the context of a three-phase system comprising fluidized sand (phase $s$), fluidized biomass (phase $b$), and gas (phase $g$) as well as of a simplified sand-gas system. The particular system use is commented in Section 4. All considered phases are treated as Newtonian fluids. The motion of the solid and gas phases is governed by the laws described below.

2.1. Governing relations. The mass conservation equation for phase $i$, which generally stands for each of the phases $s$, $b$, or $g$, reads

$$\frac{\partial (\alpha_i \rho_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i \vec{v}_i) = 0,$$

where $\alpha_i [-]$ is the volume fraction of phase $i$, $\rho_i \,[\text{kg} \, \text{m}^{-3}]$ is the density of phase $i$, and $\vec{v}_i \,[\text{m} \, \text{s}^{-1}]$ is the velocity of phase $i$.

Consequently, with regard to the considered phenomena, a basic form of the momentum conservation equation of phase $i$ reads

$$\frac{\partial (\alpha_i \rho_i \vec{v}_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i \vec{v}_i \otimes \vec{v}_i) = -\alpha_i \nabla P + \nabla \cdot T_i + \alpha_i \rho_i \vec{g} + \sum_{p \in \{s,b,g\}, p \neq i} K_{pi} (\vec{v}_p - \vec{v}_i),$$

where $P \,[\text{Pa}]$ is the gas phase pressure shared by all phases, $\vec{g} \,[\text{m} \, \text{s}^{-2}]$ is the gravity acceleration vector, $K_{pi} \,[\text{kg} \, \text{m}^{-3} \, \text{s}^{-1}]$ is the coefficient of momentum exchange between phases $i$ and $p \in \{s,b,g\}, p \neq i$, and $T_i \,[\text{kg} \, \text{m}^{-1} \, \text{s}^{-2}]$ is the stress tensor of phase $i$, which reads

$$T_i = \alpha_i \mu_i \left( \nabla \vec{v}_i + (\nabla \vec{v}_i)^T - \frac{2}{3} \nabla \cdot \vec{v}_i I \right),$$

where $\mu_i \,[\text{kg} \, \text{m}^{-1} \, \text{s}^{-1}]$ is the dynamic viscosity of phase $i$. In the case of turbulent flows, the right-hand side of equation (2) additionally includes a turbulent dispersion force term. For simplicity, we omit it in the equations although we utilize turbulence models in some of the simulations. Particular expressions of the turbulent dispersion as well as more general forms of the momentum balance for individual phases attending multiphase flows can be widely found in the literature (e.g. \cite{7}). In the case of granular flows, the right-hand side of the momentum equation for solid phase $j \in \{b,s\}$ is additionally endowed with term $-\nabla P_j$, where $P_j$ is the solids pressure.

All the phases obey laws based on the aforementioned relations. The gas phase is treated as an ideal gas. The stresses, viscosity, and pressure of the solid phases arise from granular kinetic theory (e.g. \cite{7}) and particular expressions can be found in \cite{1}.
2.2. Drag models. Here, two gas-solid momentum exchange (coefficient) models are discussed. They utilize the relative Reynolds number $Re_j$ for solid phase $j$, $j \in \{s, b\}$, defined as

$$Re_j = \frac{\rho_g \| \vec{v}_g - \vec{v}_j \| d_j}{\mu_g},$$

where $d_j$ is the (mean) diameter of particles of phase $j$. Despite being part of the models, the momentum exchange between the solid phases (see e.g. [1]) has negligible effect due to assumed small volume fractions of the solid phases. Therefore, the details on the respective terms are not included in the text.

First, the Syamlal–O’Brien model [13, 9] is used, where

$$K_{jg} = \frac{3 \alpha_j \alpha_g \rho_g}{4 \nu_{r,j}^2 d_j} C_D \| \vec{v}_j - \vec{v}_g \|, \quad C_D = \left( 0.63 + 4.8 \sqrt{\frac{\nu_{r,j}}{Re_j}} \right)^2,$$

and where

$$\nu_{r,j} = 0.5 \left( A - 0.06Re_j + \sqrt{(0.06Re_j)^2 + 0.12Re_j(2B - A) + A^2} \right),$$

$$A = \alpha_g^{4.14}, \quad B = \begin{cases} 0.8 \alpha_g^{1.28} & : \alpha_g \leq 0.85 \\ \alpha_g^{2.65} & : \alpha_g > 0.85 \end{cases}.$$  

Next, the Gidaspow model [7, 9] is considered, where

$$K_{jg} = \begin{cases} \frac{3}{4} C_D \frac{\alpha_j \alpha_g \rho_g d_j}{\nu_{r,j}^2} \alpha_g^{-2.65} & : \alpha_g > 0.8 \\ 150 \frac{\alpha_g^2 \mu_g}{\alpha_g d_j^2} + 1.75 \frac{\rho_g \alpha_j \| \vec{v}_j - \vec{v}_g \|}{d_j} & : \alpha_g \leq 0.8 \end{cases},$$

and where

$$C_D = \begin{cases} \frac{24}{\alpha_g Re_j} \left[ 1 + 0.15(\alpha_g Re_j)^{0.687} \right] & : \alpha_g Re_j < 1000 \\ 0.44 & : \alpha_g Re_j \geq 1000 \end{cases}.$$  

3. Configuration. Geometry of the combustion chamber and phase properties are taken similar to [11]. We consider a cylindrical combustion chamber with dimensions shown in Fig. 1. The gas and solid phases are allowed to enter the chamber through its inlet located on the bottom horizontal boundary, and they are allowed to escape the chamber through its outlet located on the upper horizontal boundary. For the whole duration of the simulations, constant temperature $T = 1000$ K is prescribed. In order to investigate the differences between the fluidized flow observed in the experiment using fluidization by the air and that corresponding to the oxyfuel combustion scenario, we use two different gases in our computations. The first gas corresponds to the dry air, and its volume composition is 78% N$_2$, 21% O$_2$, and 1% other components (noble gases, CO$_2$, ...). The second gas is composed of 25% O$_2$ and 75% CO$_2$ and imitates gases occurring in oxyfuel combustion regimes. For simplicity, both sand and biomass particles are considered spherical (their sphericity is 1). Phase properties used in the computations carried out in this paper are summarized in Tab. 1.
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Temperature \( T = 1000 \text{ K} \)

Air – density \( \rho_g = 0.3564 \text{ kg m}^{-3} \)

Air – dynamic viscosity \( \mu_g = 4.1923 \cdot 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1} \)

Oxyfuel gas – density \( \rho_g = 0.495 \text{ kg m}^{-3} \)

Oxyfuel gas – dynamic viscosity \( \mu_g = 5.8227 \cdot 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1} \)

Sand – particle diameter \( d_s = 0.78 \text{ mm} \)

Sand – density \( \rho_s = 2655 \text{ kg m}^{-3} \)

Sand – dynamic viscosity \( \mu_s = 0.5 \text{ kg m}^{-1} \text{ s}^{-1} \)

Sand – packing limit 0.59

Biomass (Miscanthus) – particle diameter \( d_b = 10.36 \text{ mm} \)

Biomass (Miscanthus) – density \( \rho_b = 603 \text{ kg m}^{-3} \)

Biomass (Miscanthus) – dynamic viscosity \( \mu_b = 0.5 \text{ kg m}^{-1} \text{ s}^{-1} \)

Biomass (Miscanthus) – packing limit 0.5

Table 1. Phase properties corresponding to given temperature and gas composition (air, oxyfuel). Diameter \( d_b \) is calculated so that the volume of a particle corresponds to the average volume of biomass pellets used in [11]. Note that the kinematic viscosity values of all the phases have the same order of magnitude (\( \propto 10^{-4} \text{ m}^2 \text{ s}^{-1} \)).

3.1. Initial and boundary conditions. The simulations start with the empty combustion chamber. At the inlet, we prescribe the mass inflow rates of all the phases as well as the phase velocity ratio. The ratio of the solid particles velocities to the gas velocity is 0.01. This setup of the numerical simulations allows us to study the fluidization processes because the particles enter the chamber with low velocity and get transported by the flowing gas due to the momentum exchange. At the outlet, the pressure outlet condition is prescribed. The no-slip condition is used at the remaining walls of the combustion chamber.

Two different sand fluidization regimes are considered:

- Bubbling – The gas mass inflow rate is 0.02912 kg s\(^{-1}\).
- Circulating – The gas mass inflow rate is 0.07275 kg s\(^{-1}\).

In both regimes, the mass inflow rate of sand and biomass is 0.15 kg s\(^{-1}\) and 0.00083 kg s\(^{-1}\), respectively. These values of the solid mass rates approximate the corresponding mass inflow rates of the steady state flow in the case of the circulating regime. Hence such setup represents a simple model of solids recirculation in the circulating regime. Boundary conditions for biomass were calculated to give the mass flux approximately 5 kg h\(^{-1}\), which is value taken from [11].

4. Numerical solution.

4.1. ANSYS Fluent. ANSYS Fluent is an engineering simulation software based on the finite volume method. The Eulerian multiphase model for 3 phases with
Figure 1. Dimensions of the combustion chamber and meshes considered. (A) Dimensions of the cross-section of combustion chamber. (B) Coarse mesh generated by ANSYS Meshing. (C) Cross-section of the mesh in ANSYS. (D) Cross-section of the mesh in OpenFOAM generated by BlockMesh.

an implicit formulation in time was used. The time step was $\Delta t = 0.001 \text{ s}$ for all simulations. Laminar viscous model was used. Gas, bed material, and pellets of miscanthus were represented by a fluid material with different densities and dynamic viscosity.

Computational domain was discretized by the finite mesh generated by ANSYS Meshing (a part of the ANSYS software package) as depicted in Fig. 1. It was experimentally verified (by using finer meshes) that the chosen mesh resolutions were sufficient for producing consistent results in the circulating regime. For the computation the fixed time stepping method with maximal 20 iterations per time step is used.

4.2. OpenFOAM. OpenFOAM is an open-source framework for the development of solvers in computational fluid dynamics. It includes many pre-implented solvers for various applications, two of which were used for the simulations in this paper. The solver `twoPhaseEulerFoam` was set up to solve a dispersed two-phase flow (gas and solids), and the solver `reactingMultiphaseEulerFoam` was set up to solve a dispersed three-phase flow (gas, solids, and biomass), without any reactions. The phase properties from Tab. 1, initial and boundary conditions from Sections 3.1 were used in both solvers. The reason for comparing results produced by these two solvers is that while `reactingMultiphaseEulerFoam` allows solving a general multiphase model, `twoPhaseEulerFoam` contains more turbulence models, including a model based on particle-phase pressure [7]. As will be seen from the results, the turbulence model has an important role in the setup considered in this paper.

The computational mesh whose cross-section is depicted in Fig. 1 is described in the `blockMeshDict` format. In the solver `twoPhaseEulerFoam` a constant time-step $\Delta t = 2 \cdot 10^{-4} \text{ s}$ was used and in the solver `reactingMultiphaseEulerFoam` an
adaptive time stepping with maximum $\Delta t = 10^{-3}$ s and maximum Courant number $Co = 0.5$ was used.

4.3. CFBSim. CFBSim is a quasi-1D solver originally developed for biomass co-firing in a circulating fluidized bed boiler. The employed model is based on the work of Gidaspow [7] and it was developed for industrial purposes in collaboration with Honeywell corp. (see [4]). For the purpose of this paper, it was modified for the geometry of the combustion chamber depicted in Fig. 1 and equations responsible for combustion processes were deactivated. The model solves Euler equations [4] instead of Navier-Stokes equations described in Mathematical model section. All conservative laws are reformulated in 1D along the vertical profile of the combustion chamber and its horizontal variable cross-section denoted by $A(x)$, where $x$ is the elevation, is taken into account.

The resulting governing equations are spatially discretized using finite volume scheme on a uniform mesh. The time integration is provided by the fourth order Runge–Kutta–Merson method with the adaptive time stepping [6].

5. Numerical results. In this section, we present and compare the computational results of the models discussed in Section 4. The CFBSim solver is only used in the circulating fluidization regime for which it was designed. Simulation parameters are summarized in Tab. 1. For 3D simulations, the relevant quantities are averaged over the cross-section of the combustion chamber and the resulting 1D profiles along the vertical axis are compared and analyzed. The velocity of each phase $i$ is averaged as

$$\frac{\int_{S_y} \alpha_i \vec{v}_i dS}{\int_{S_y} \alpha_i dS},$$

where $S_y$ is the cross-section of the combustion chamber at height $y$, and the linear density is calculated as

$$\int_{S_y} \alpha_i \rho_i dS.$$

5.1. Bubbling regime. In the bubbling regime, the gas phase forms bubbles bounded by solid particles clumped together. This persists as long as the gas has enough momentum to lift particles up. As shown in Fig. 3, the average gas velocity decreases in the widening of the chamber which leads to the violation of conditions for the bubble formation and the subsequent fall of the solid particles back to the narrow part of the chamber. The illustrative result demonstrating the dynamics of sand particles in the bubbling regime is shown in Fig. 2.

5.2. Circulating regime. In the circulating regime, ANSYS Fluent, OpenFOAM and 1D CFBSim all used the Gidaspow drag model unless otherwise noted. In all three cases, the steady state for the gas and sand phases was reached quickly. All following results are visualized at time $t = 3$ s when the steady state was already reached. In the case of gas velocity, Fig. 3 shows very good agreement of all three studied models.

Results comparing the dynamics of sand particles are depicted in Figs. 4 and 5, where the linear densities and velocities of sand particles are plotted, respectively. These results show that in the case of circulating regime, both ANSYS Fluent and OpenFOAM provide very good agreement. However, it can be seen that 1D code CFBSim exhibits very different behavior. The differences between the 1D and 3D cases may be attributed to the differences in the implementation details,
e.g., both ANSYS Fluent and OpenFOAM use point-wise values of velocities in the evaluation of the drag coefficient instead of averaged values, which would allow better comparison with the 1D model. Moreover, the comparison was influenced by several effects which can not be completely incorporated in a 1D model, such as the interaction with walls, added turbulence model or different velocity distribution over the cross section of the combustion chamber.

As expected, results from the 1D CFBSim solver differ from averages provided by 3D models and the lower magnitude of the velocity is in agreement with, e.g., the higher linear density - see Figs. 4 and 5. Here, it can also be seen that in the widened part of the chamber, there is a difference between ANSYS Fluent and OpenFOAM. Such slight differences between OpenFOAM and ANSYS Fluent are caused by different regularizations of the solid particle drag models in both software packages. Similarly, the comparison of the velocity and linear density of biomass
is plotted in Figs. 6 and 7. While in the case of 1D CFBSim code, the flow of biomass particles reaches the steady state and the circulation regime for biomass is established, in ANSYS Fluent there is a chaotic behavior in the lower part of the chamber and the steady state is never reached. For ANSYS Fluent it was possible to perform the comparison between the drag models according to Gidaspow [7] and Syamlal [13], and the comparison of velocities is depicted in Fig. 8 and the comparison of sand linear densities is depicted in Fig. 9. Numerical data from this experiment show a decent qualitative agreement between both models and approach towards the agreement with the OpenFOAM model.

The \texttt{twoPhaseEulerFoam} solver from the OpenFOAM package supports many turbulence models. The comparison of linear densities and velocities of sand particles for a laminar model and a Reynolds–averaged simulation (RAS) using the \( k - \epsilon \) turbulence model [8] for the gas phase and a turbulence model based on phase-pressure [7] for the sand particles phase is shown in Figs. 10 and 11. In the laminar case, there is higher volume fraction of sand particles near the wall in the upper part of the combustion chamber. The \( y \)-component of the velocity is negative there, which causes a significant drop in the averaged velocity profile compared to RAS. Compared to the 1D model, the velocity profile in the laminar case approaches the 1D profile in the bottom part of the chamber. On the other hand, as has been shown in Fig. 5, the velocity profile for the RAS model agrees with the results from ANSYS Fluent. This suggests that the appropriate choice of the turbulence model has a significant effect on the results in the considered configuration of the model.

Unlike the \texttt{twoPhaseEulerFoam} solver, the \texttt{reactingMultiphaseEulerFoam} solver from the OpenFOAM package does not support the turbulence model based on particle-phase pressure. Hence, only the laminar three-phase model can be considered for comparison with other models. The linear densities and velocities of solid and biomass particles in the three-phase model are compared with the results of the two-phase model in Figs. 12 and 13. It can be seen that the linear density of biomass is significantly lower compared to the sand particles and it stays in the bottom part of the chamber in the bubbling regime due to low velocity, so the
problems discussed in Sec. 5.1 apply. Since the presence of biomass has a negligible effect on the other phases, the differences between the profiles for sand particles are most likely caused by subtle differences in the implementation of the models.

Finally, the dependence of the flow profiles on the used gas (oxyfuel flue gas vs. air) is presented in Figs. 14, 15 and 16, where the gas velocity, sand particles velocity, and the linear density of sand particles are plotted, respectively.

![Figure 4](image1.png)

**Figure 4.** Linear density of sand particles along the vertical axis of the combustion chamber. Circulating regime.

![Figure 5](image2.png)

**Figure 5.** Velocity of sand particles averaged across the cross-section of the chamber. Circulating regime.

6. **Conclusion.** The presented work is the first step in an ongoing effort to develop a complex CFD model of hydrodynamics, combustion, heat transfer and pollutant production in oxyfuel fluidized bed boilers. We investigated the capabilities and behavior of three different implementations of fluidization models. The study revealed that in the bubbling regime, the process is extremely chaotic and every subtle detail of the model influences the results. To assess the individual models in this regime, a statistical analysis of the flow would be appropriate, which has not yet been performed.
In the circulating regime, solids recirculation was approximated by prescribing a constant solids inflow at the inlet. The model comparison showed that three-dimensional effects such as turbulence and velocity distribution along the cross-section of the combustion chamber play an important role. The quasi-1D model, which is naturally only applicable to the circulating case, produces results that deviate significantly from both 3D models. The quasi-1D simplification will therefore be excluded from the further development of the model. On the other hand, it turned out that the flow with more granular materials (sand and biomass) can be solved separately for each of them as long as their volume fractions remain low.

Although combustion and heat transfer effects are not taken into account yet, it is already apparent from the results that flue gas composition in oxyfuel combustion largely influences the nature of the flow. In further collaboration with the experimentalists involved in the project acknowledged below, the modeling result
Figure 8. Velocity of sand particles averaged across the cross-section of the chamber in circulating regime for Gidaspow [7] and Syamlal [13] drag models.

Figure 9. Linear density of sand particles in circulating regime in dependence on drag models according to Gidaspow [7] and Syamlal [13].

will therefore be helpful for tuning the device setup from the viewpoint of hydrodynamics.

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Figure 11. Comparison of the profiles of the velocity of sand particles averaged over the cross-section of the chamber obtained using the RAS turbulence model and laminar flow model available in the OpenFOAM package (solver twoPhaseEulerFoam). The profiles are also compared with the velocity profile obtained by the 1D CFBSim model.

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Figure 13. Comparison of particle velocities averaged over the cross-section of the chamber in the two-phase laminar model (OpenFOAM solver \texttt{twoPhaseEulerFoam}) and three-phase laminar model (OpenFOAM solver \texttt{reactingMultiphaseEulerFoam}).

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Figure 14. Comparison of the gas velocity averaged over the cross-section of the chamber under the oxyfuel setting and the air setting. Computed in ANSYS Fluent.

Figure 15. Comparison of the velocity of sand particles averaged over the cross-section of the chamber under the oxyfuel setting and the air setting. Computed in ANSYS Fluent.

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Figure 16. Comparison of the linear density of sand particles under the oxyfuel setting and the air setting. Computed in ANSYS Fluent.