DEVELOPMENT OF AN OPENFOAM SOLVER FOR NUMERICAL SIMULATION OF CARBONIZATION OF BIOMASSES IN ROTARY KILNS

SALAR TAVAKKOL[1], THORSTEN ZIRWES[2], JORDAN A. DENEV[3], FARSHID JAMSHIDI[4], HENNING BOCKHORN[5]

[1]*Engler-Bunte-Institute, Karlsruhe Institute of Technology, Karlsruhe, Germany, Salar.Tavakkol@kit.edu*

[2]*Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Karlsruhe, Germany, Thorsten.Zirwes@kit.edu*

[3]*Steinbuch Centre for Computing, Karlsruhe, Karlsruhe Institute of Technology, Germany, Jordan.Denev@kit.edu*

[4]*Institute of Digital Materials Science, University of Applied Sciences, Karlsruhe, Germany, Farshid.Jamshidi@hs-karlsruhe.de*

[5]*Engler-Bunte-Institute, Karlsruhe, Karlsruhe Institute of Technology, Germany, Henning.Bockhorn@kit.edu*

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Abstract

Carbonization is a key process to increase the energy density of high moisture containing biomasses and biogenic wastes and to provide multi-purpose raw chemicals for further applications. Steam assisted carbonization is a kind of slow pyrolysis, in which wet biomass is treated continuously in superheated steam at elevated temperature and atmospheric pressure. Rotary kiln reactors due to their flexibility and easy control of operating conditions are well suited for this process. In this work a numerical simulation tool based on an Eulerian-Langrangian approach has been developed to simulate the carbonization of biomasses in rotary kiln reactors resolved in time and space by combining existing OpenFOAM features and developing new physical models. This study demonstrates the features of this extended and validated Eulerian-Lagrangian approach for simulating dense particulate multiphase flows in large-scale rotary kiln reactors. The focus is to using the new tool to aid the design of large scale rotary kiln reactors by performing parameter studies. The simulations of this kind of large scale reactors require large computational resources on supercomputers. Therefore, a further focus lies in different approaches to reduce the computational effort while keeping the accuracy at an acceptable level. By using the MP-PIC model, computing time increases linearly with the number of biomass particles instead of exponentially with the DPM model. The optimal cell size has been found to be about twice the largest particle diameter. By choosing the optimal domain decomposition method, simulation time can be reduced by a factor of 1/10. Introducing a solver frequency parameter to the DOM radiation model can help to reduce simulation times further by a factor of 1/8 while decreasing the accuracy by only 2%. Parallel scaling tests show good performance with over 1000 CPU cores. These results show that simulations with a total of 40,000 CPU-hours per studied case become feasible proving the developed solver to be an efficient tool for the design of rotary kiln reactors.

Introduction

In times of dynamic changes in energy supply and with continuing efforts to reduce the impact on environment, new resources and new technologies are exploited to meet the high future demands. One example is the utilization of biomasses, which after compaction of energy can serve as energy carrier or multi-purpose raw chemical. Carbonization increases the energy density of wet biomasses or bio wastes and, therefore, is a process to be considered in this context. The present work focuses on modeling the continuous carbonization of wet biomasses in rotary kiln reactors. The targeted reactors work with superheated steam evaporated from the biomass at atmospheric pressure and elevated temperatures up to 873 K. Under these conditions, the biomass undergoes a process of steam-assisted carbonization [1]–[4].

Numerical simulation of carbonization of biomasses, which can be performed at different operating conditions [5], requires two-phase modeling capabilities. Lagrangian methods allow tracking of individual biomass particles and, therefore, the treatment of the heat-, mass- and chemical conversion processes of each particle [6] as well as their interaction with the surrounding fluid phase. In the present work, a newly developed simulation tool is utilized to simulate large scale rotary kiln reactors. The tool is based on OpenFOAM and uses a Lagrangian approach known as Multi-Phase Particle-In-Cell (MP-PIC) model from O'Rourke et. al. [7], [8] with an isotropic particle stress gradient model from Harris and Crighton as the core of particle-particle interaction [9]. This model is available in OpenFOAM [10], however, justified only for isothermal conditions and incompressible formulation of the Navier-Stokes equations [11], [12]. The newly developed tool extends the use of the collision model to compressible reacting flows and provides four-way-coupling between the gas and particulate phase. For the Lagrangian particles, constituted by multicomponent biomass particles, an

energy equation is solved. The modified solver enables calculating flows with any particle volume fraction from the dilute to the close-pack limits in the rotary kiln and includes coupling of heat and mass transfer between phases. For the gas phase, an Eulerian method solves the Navier-Stokes equations in compressible formulation, the energy equation and the balance equations for chemical species considering drying and devolatilization of the particulate phase.

Additional constituents of the model have also been improved to describe more properly the physical and chemical processes in rotary kiln reactors. For the radiative heat transfer an adjustment for the existing discrete ordinate model (DOM) is introduced to consider the shadowing of particles. The high moisture content in the biomass feedstock can create fully saturated or pure steam conditions in the freeboard gas. For this condition, existing vaporization models in OpenFOAM, which are based on diffusion controlled and flash-boil vaporization, need to be extended to describe constant temperature vaporization. Furthermore, an n-th order kinetic devolatilization model is implemented in OpenFOAM for the modeling of devolatilization based on the experimental work of Bockhorn et. al. [13]–[15]. The validation of the extended numerical model has been performed by a series of simulations of a laboratory-scale rotary kiln for spherical and non-spherical biomass particles [16],[17]. Residence time, mixing degree, convective and radiative heat transfer and devolatilization are validated against experiments in a previous work [16].

The newly developed simulation tool for the carbonization of wet biomasses in large scale rotary kiln reactors requires large computational resources, which are more than two orders of magnitude higher compared with the simulation of laboratory scale reactors from previous works [16]. Therefore, the numerical efficiency of each part of the model has to be ensured and the workload has to be balanced between many CPU cores on big supercomputers. This is especially important when applying this tool in series of simulations to find optimal process conditions for large scale reactors. Therefore, an additional focus of this work is to demonstrate the possibility of the simulation of large scale reactors by achieving a satisfactory balance between accuracy and computational effort.

Physical Modeling and Implementation

Carbonization of biomass in rotary kiln reactors comprises heating up the solid due to heat exchange with the hot gas phase and radiation from the hot reactor walls. By heating up moisture evaporates to the gas phase and at sufficiently high temperature chemical carbonization process occurs. During that process, the biomass particles form a bed inside the reactor and particles interact by collision.

OpenFOAM provides many of the required models for the above mentioned physical/chemical processes and can easily be extended because of its modular structure. However, some key aspects are missing and had to be added to the existing structure. For the Langrangian treatment of particles which requires the position, velocity, thermodynamical state and chemical composition of each particle, a module without considering particle collisions is contained in OpenFOAM. Using OpenFOAM's class templates which allows to create a new Lagrangian particle type as a combination of OpenFOAM's ReactingMultiphaseParcel type and CollidingParcel type, a new particle type has been introduced which is capable of both the thermo-chemical processes as well as packed bed formation. In this way, the four way coupling between gasphase and particles can be realized. The collision model can be chosen to the discrete particle model (DPM) [18] or the multiphase particle in cell model (MP-PIC) [19]. Movement of the Lagrangian particles is computed from

$$\frac{\mathrm{d}\boldsymbol{x}_\mathrm{p}}{\mathrm{d}t} = \mathbf{v}_\mathrm{p}, \quad m_p \frac{\mathrm{d}\mathbf{v}_\mathrm{p}}{\mathrm{d}t} = \sum_i \boldsymbol{F}_i,$$

where t is time, x_p the particle's positions, $\mathbf{v}_p$ its velocity and $\boldsymbol{F}_i$ forces like drag, gravity, particle-particle and wall-particle interaction forces. The particles temperature is computed from

$$m_\mathrm{p} c_{p_\mathrm{p}} \frac{\mathrm{d}T_\mathrm{p}}{\mathrm{d}t} = \dot{Q}_\mathrm{conv} + \dot{Q}_\mathrm{rad} - \dot{Q}_\mathrm{evap} - \dot{Q}_\mathrm{devol},$$

where c_{p_p} is the isobaric specific heat capacity of the particle, T_p its temperature, $\dot{Q}_\mathrm{conv}$ the convective heat flux by heat transfer with the gas phase, $\dot{Q}_\mathrm{rad}$ the heat flux due to radiation, $\dot{Q}_\mathrm{evap}$ the energy change during evaporation and $\dot{Q}_\mathrm{devol}$ the net heat flux due to devolatilization during the carbonization process.

The models for radiation, evaporation and devolatilization have been modified to work for the physical conditions commonly found in rotary kiln reactors. While the biomass particles heat up and reduce their moisture content due to evaporation, the gas phase within the reactor can be saturated with water vapour. Therefore, the existing evaporation models of OpenFOAM have been extended to work in saturated atmospheres and also to consider evaporation below the boiling temperature. For the devolatilization, a new model has been implemented based on an experimental correlation [13]–[15]. This assumes a global chemical reaction where the reaction rate is modeled as an n-th order Arrhenius kinetic rate law. The activation energy of this global reaction is determined experimentally and averaged for the volatile components water, tar, carbon dioxide and carbon monoxide. Lastly, the raditation model was extended to take the radiative shielding between the particles into account. Because the particles form a packed bed, radiative heat transfer from the hot reactor walls occurs mostly with the outermost layer of biomass particles. Based on the discrete ordinates

model (DOM), the developed radiation model computes the absorption coefficient in each computational cell based on the volume fraction of Lagrangian particles. For more information about the introduced physical models and their validation, see [16],[17].

The simulation of the gas phase utilizes OpenFOAM's finite volume approach and is considered as an Eulerian phase consisting of nitrogen, water steam, carbon monoxide, carbon dioxide and tar. The balance equations for mass, momentum, energy and chemical species are:

$$\frac{\partial \rho_\mathrm{g}}{\partial t} + \nabla \cdot \left(\rho_\mathrm{g} \boldsymbol{u}_\mathrm{g}\right) = S_{\mathrm{p},m} \,,$$

$$\frac{\partial \rho_\mathrm{g} \boldsymbol{u}_\mathrm{g}}{\partial t} + \nabla \cdot \left(\rho_\mathrm{g} \boldsymbol{u}_\mathrm{g} \boldsymbol{u}_\mathrm{g}\right) = -\nabla p + \nabla \cdot \tau + \rho_\mathrm{g} \boldsymbol{g} + \boldsymbol{S}_{\mathrm{p},mom} \,,$$

$$\frac{\partial \rho_\mathrm{g} h}{\partial t} + \nabla \cdot \left(\boldsymbol{u}_\mathrm{g} \rho_g h\right) = \nabla \cdot \left(\rho_g a \nabla h_\mathrm{s}\right) + \frac{\partial p}{\partial t} + S_{\mathrm{p},h} + S_\mathrm{rad} \,,$$

$$\frac{\partial \rho_\mathrm{g} Y_i}{\partial t} + \nabla \cdot \left(\rho_\mathrm{g} \boldsymbol{u}_\mathrm{g} Y_i\right) = \nabla \cdot \left(\rho_\mathrm{g} D_i \nabla Y_i\right) + S_{\mathrm{p},Y_i} \,,$$

where, ρ_g is the gas phase density, $\boldsymbol{u}_\mathrm{g}$ its velocity, p the pressure, τ the stress tensor which considers turbulent fluctuations with the Smagorinsky turbulence model and $\boldsymbol{g}$ is the gravitational acceleration. h is the total enthalpy of the gas, h_s its sensible enthalpy and a its thermal diffusivity. Y_i is the mass fraction of the i-th species and D_i its diffusion coefficient. The source terms S_p enable the exchange of momentum, energy and chemical species between the gas phase and the Lagrangian biomass particles.

Numerical Setup

The goal of the newly developed simulation tool is to aid the design of large scale reactors for biomass carbonization. The numerical mesh consists of a cylinder with a length of 12 m and a diameter of 1.2 m.

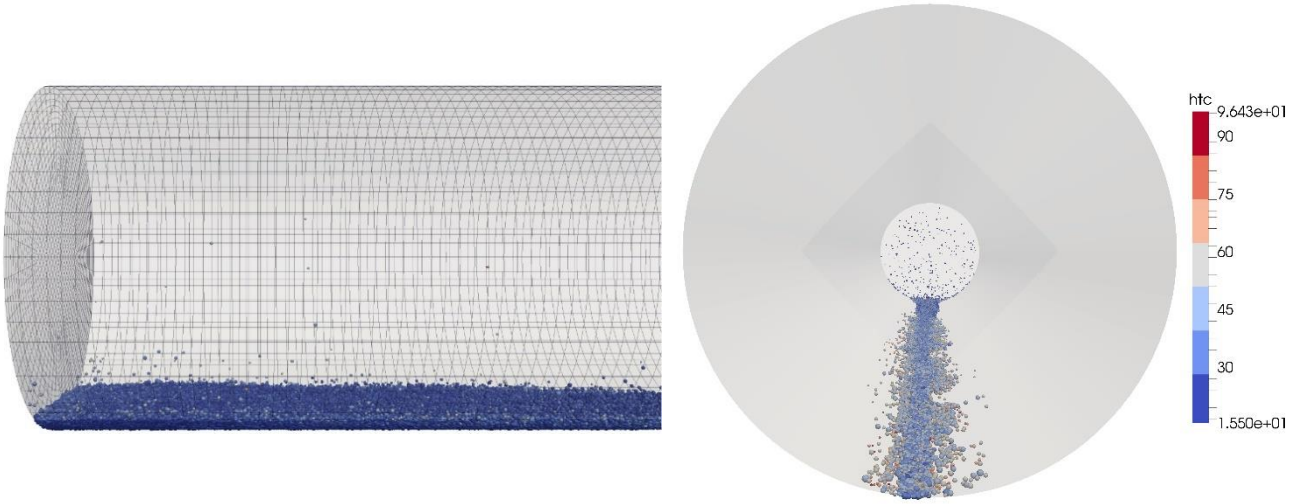

Figure 1: Side view (left) and frontal view (right) of the cylindrical mesh of the reacor. Biomass particles are colored by their heat transfer coefficient (htc) in W/(m²K).

Figure 1 on the left shows the cylindrical mesh of the reactor near the inlet patch. The biomass particles are injected from the inlet patch and move along the reactor. The reactor rotates with 10 revolutions per minute and wall temperatures are set between 673 K and 973 K, depeding on the case being examined. The whole reactor is tilted with an inclination angle between 0.5° and 2°. The biomass particles form a bed at the bottom of the reactor, as shown in **Figure 1** on the left. In **Figure 1** on the right, a frontal view at the outlet of the reactor is given. The inlet plane is in the back where the biomass particles are injected into the reactor. The particles are colored by their heat transfer coefficient (htc). More information about the setup can be found in [16],[17].

The number of Lagrangian particles representing the biomass particles required to accurately represent the real kiln process exceeds millions of particles, with hundred of thousands to millions of particles being in the reactor simultaneously. On the other hand, the number of computation cells in the mesh must be fine enough to resolve the interaction between the particles and the gas phase. Lastly, the simulation time step is limited by the CFL condition to be

of the order of 3 – 10 milliseconds while the average residence time of the particles inside the reactor is approximately 2700 seconds. Because of this, simulation of such a reactor on a large scale is only possible on high performance computers. Nevertheless, compromises between grid resolution, number of particles and solver settings are necessary to obtain accurate results while keeping the computational resources feasible.

Result and discussion

For finding of the kind of compromise mentioned above, a grid dependence study has been performed in this work. The finest computational mesh considered consists of 2,700,000 hexahedral control volumes with an average edge size of 2 cm. The total length of the reactor is 12 m. This is the finest possible mesh resolution due to the restriction from particle volume fractions in a cell because the largest biomass particles have a diameter of about 2 cm. Coarser meshes with an average edge size of 4×4×4, 8×8×8, 10×10×10 cm are composed of 375,000, 48,000 and 21,600 cells, respectively. Another possibility to reduce the mesh size is to coarsen the cells only in the axial direction and therefore to keep the radial distribution as fine as possible. Therefore, mesh resolutions with average edge sizes of 2×2×5 and 2×2×10 cm have also been studied.

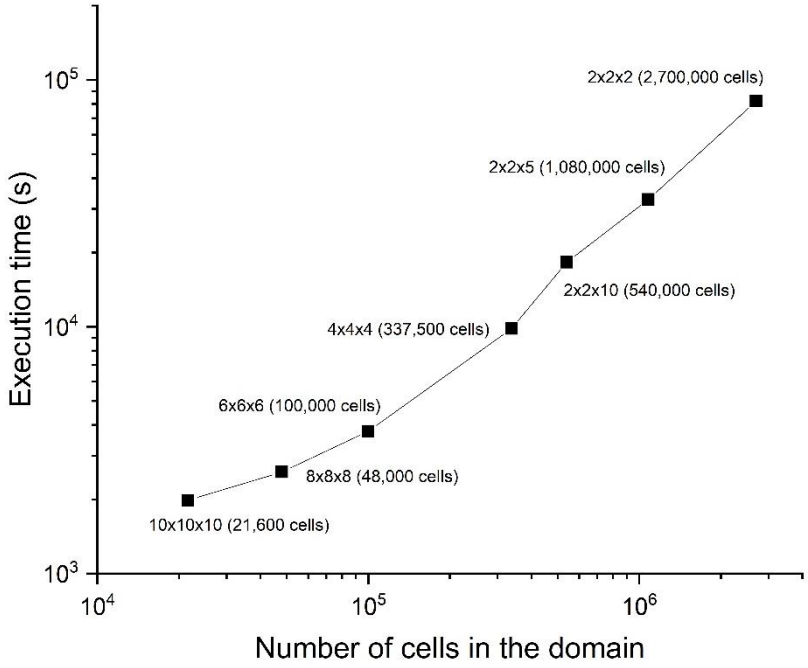

Figure 2: Overall performance of the simulation using different grid sizes.

Figure 2 shows that the execution time of the simulation increases roughly linearly with the number of cells. In order to decide which grid resolution is sufficient, results of the calculated gas temperature on the centerline of the reactor with various grid sizes from **Figure 2** are shown in **Figure 3**. The temperatures are time averaged over the first 230 s of simulation time. By comparing the finest mesh with the 4×4×4 cm case, the relative deviation in time-averaged gas temperatures at the centreline of the reactor is only about 0.30%. The 4×4×4 cm grid accelerates the simulation by a factor of 8.45 with an acceptable deviation. The mesh with average edge sizes of 2×2×5 also exhibits an acceptable precision especially at the inlet region of the reactor but the simulation is still expensive for long runs. On the other hand, the precision of the axially coarsened mesh with 2×2×10 cm cells is not better than that of the 4×4×4 cm cell grid despite the higher cell number. This emphasizes that the aspect ratio of cells is a decisive factor of the precision in the simulation. In this study, the grid with an average size of the 4×4×4 cm is chosen for the large-scale simulation as a compromise between precision and performance.

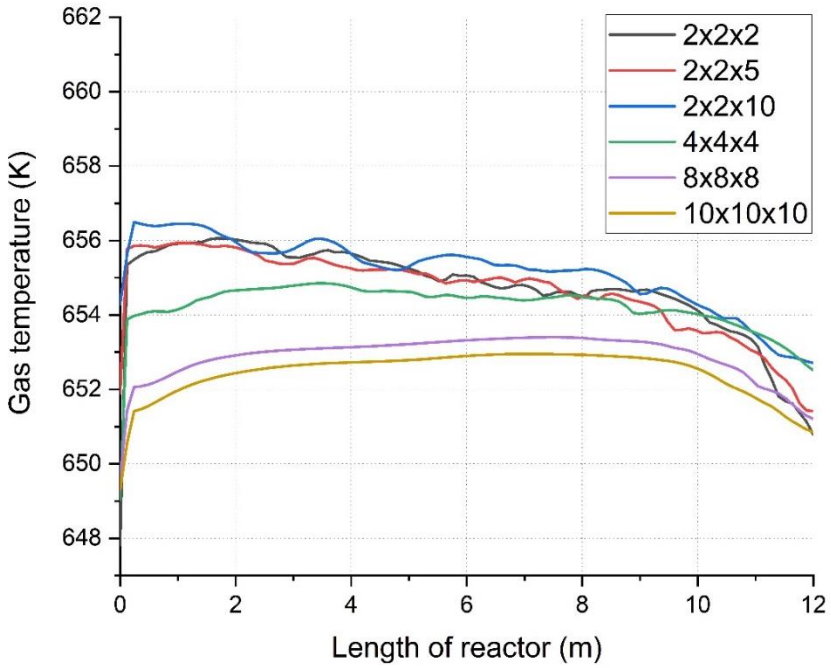

Figure 3: Gas temperature on the centreline along the reactor for different grid sizes.

Besides the grid dependence study, the influence of the number of particles in the domain on the total cpu time per time step is also studied in this work. The CPU performance for the computation of the disperse phase using the MP-PIC method is tested for a short simulation with 2 s physical time and increasing the number of particles from 5,000 to 450,000 in 11 steps. In reality, the number of particles inside the reactor is even higher. Therefore, in this work each Lagrangian parcel represents 10 biomass particles for a feasible computational performance. In the steady-state condition, there are more than 3,330,000 biomass particles in the domain at the same time. On the other hand, it was found in [16] that the computation time of the DEM-based model in the lab-scale grows exponentially with the number of particles. Even applying the reduced particle stiffness model suggested by [20] to the DEM, it is still too computationally expensive for large-scale simulations. The results from **Figure 4** show that the computational effort using the MP-PIC model increases linearly with the number of particles in the domain, so that the MP-PIC method is used for the large scale simulation. For a single CPU core, the average execution time per timestep grows from 5.1 s to 31.2 s from the smallest to the largest number of particles, respectively.

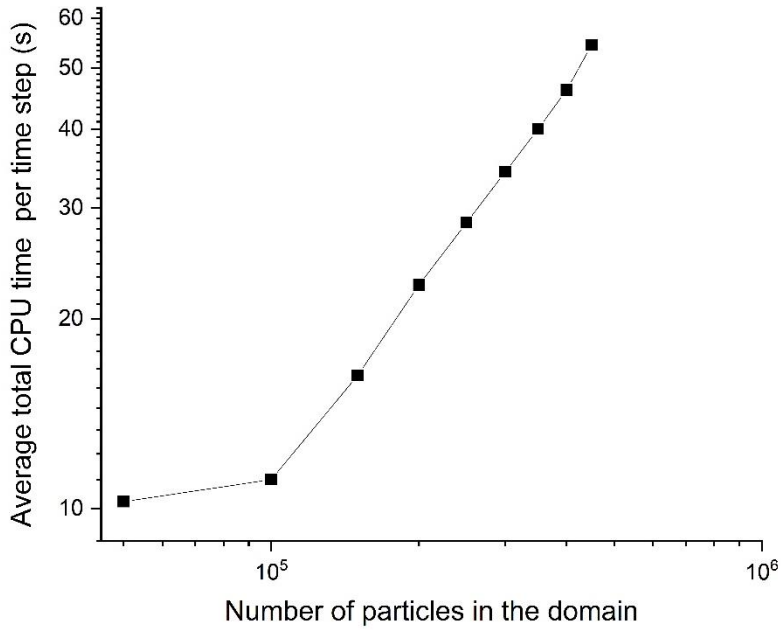

Figure 4: Performance of a single CPU by varying the number of particles in the domain.

Another significant parameter influencing the simulation performance is the domain decomposition. In the simulations including a large number of Lagrangian particles, the decomposition method has to be chosen carefully to minimize the computational effort. The Scotch decomposition method decomposes the domain based on minimizing the

interconnection between sub-domains. This helps to reduce the data exchange between processes but ignores the Lagrangian particles leading possibly to an imbalance of the number of Lagrangian particles per sub-domain. Among all available decomposition methods, it is found out that uniform decomposition in axial direction yields the best performance in the case of long-run and steady-state simulations. As shown in **Figure 1**, the particles collect at the bottom of the reactor and are distributed approximately evenly along the axial direction. The worst case decomposition is based on uniform decomposition based on the direction of the reactor height. The different approaches are shown in **Figure 4**. In A, the worst case approach is illustrated. Each color represents a sub-domain. Because all particles are located at the bottom of the reactor, only one process responsible for the bottom sub-domain has to compute all Lagrangian particles. This load increases over time as the number of particles increases in the domain. **Figure 5**B shows the uniform decomposition in axial direction, which yields the best results and C shows the decomposition with the Scotch method, which performs between the worst case A and best case B.

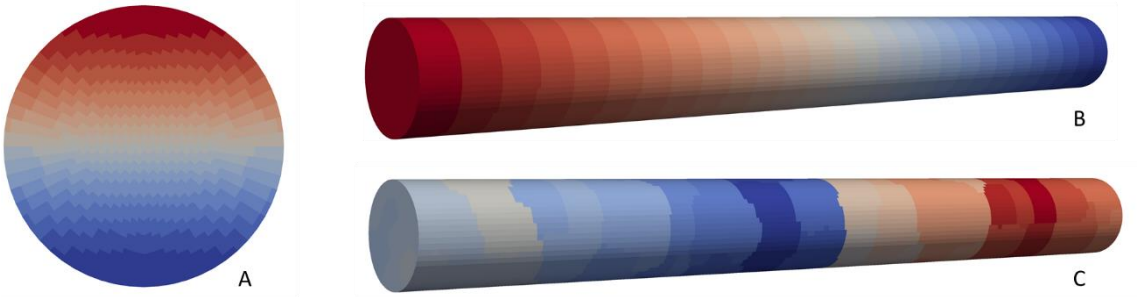

Figure 5: Different methods of decomposing the computational domain for parallel runs. Colors show the sub-domains.

Because the full simulation of the large scale reactor is only possible on massive parallel hardware, the parallel performance is tested with 2 up to 1120 CPU cores on the high-performance computer "bwUniCluster 1.0" at the Karlsruhe Institute of Technology, Germany. Reasonable parallel scaling is observed up to 560 CPU cores. The average total amount of CPU-hours for each simulated case is around 40,000. **Figure 6** represents the performance of the runs with different numbers of parallel CPU cores.

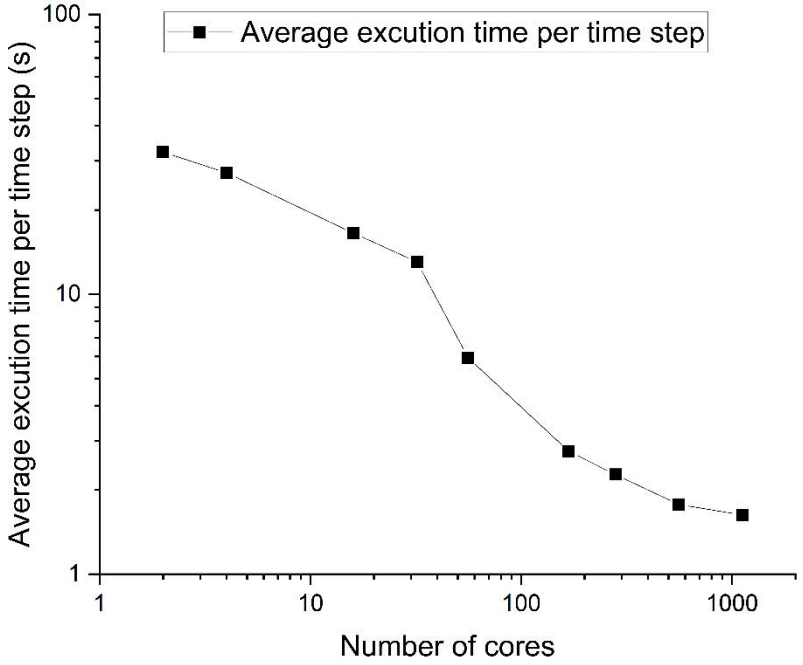

Figure 6: Execution time of the simulation, based on the number of parallel CPU cores.

The radiation model is one of the most computational intensive mathematical submodels in this work. The DOM radiation model requires setting the number of spatial directions for ray-tracing. Here, we compare the results of using 72 instead of the default 128 discrete directions. Additionally, a large portion of the simulation time can be saved, when the radiation compuations are not performed at every simulation time step. Therefore, results of calculating the radiation at every time step, every 10^{th} and every 20^{th} time step are compared (solver frequency of 10 and 20). The results are compared with the refined case with 128 directions and the solver frequency of one in **Table 1**. By introducing the solver frequency of 20 and reducing the number of discrete directions to 72, the computation time can be reduced by a factor of 1/7 while decreassing the average particle temperatures by only 2.7% . Results are obtained from runs with 16 parallel CPU cores.

Table 1: Computing time and relative deviation during a one-hour simulation in a laboratory-scale reactor.

Discrete directions	Solver freq.	Relative computation time	Relative deviation (%)
128	1	9.30	-
72	1	5.63	2.690
72	10	1.52	2.385
72	20	1.32	2.498
No Radiation	Not defined	1	Not defined

Conclusion

A new simulation tool has been developed based on the open-source framework OpenFOAM which aids the design of rotary kiln reactors for biomass carbonization. The tool treats biomass particles in a Lagrangian frame of reference and simulates the multicomponent gas phase in the reactor with the help of an Eulerian approach. OpenFOAM's capabilities are extended by allowing four-way-coupling between the gas phase and the particles by considering collisions between particles and the exchange of momentum, energy and chemical species between the gas and the particles. In addition to four-way coupling, the new tool also provides new models for the evaporation, devolatilization and radiation, all specifically tailored to the conditions commonly found in rotary kiln reactors.

Apart from the physical modeling, the main difficulty of performing simulations of large scale reactors are the computational resources. The length of the considered reactor is of the order of 10 m while the size of the biomass particles is of the order of centimeters. This results in a large number of Lagrangian particles representing the biomass particles as well as a large number of cells in the computational mesh for the Eulerian phase. Similiarly, the simulation time step is of the order of below 10 milliseconds while the process takes places on time scales of hours.

In order to make the simulations possible, different approaches are presented to drastically reduce the simulation time while keeping the accuracy of the results at an excaptable level. First, the optimal cell size has been found to be about twice the size of the largest Lagrangian particles. The aspect ratio of the cells should be close to a cube to ensure sufficient accuracy. The discrete particle model (DPM) has been found to be infeasible due to its large computational effort. Instead, it has been shown that the simulation time increases linearly with the number of particles if the MP-PIC collision model is employed. In addition to that, a ratio of ten physical biomass particles for each Lagrangian parcel has been shown to be a good balance between computing time and accuracy.

Due to the presence of the Lagrangian particles, the Scotch decomposition method has been found to be inferior to a straight forward uniform decomposition in the axial direction. Compared to uniform decomposition in radial direction, this reduces computing times to one tenth. Parallel scaling could be shown to be efficient up to over 500 CPU cores.

In conclusion, OpenFOAM has been utilized as a framework for the development of a numerical tool to enable the process optimization of large scale rotary kiln reactors. In this work we could show, that even simulations of large scale reactors are possible if the aforementioned tradeoff between computational effort and accuracy are made.

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