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INTEGRATION OF HIGH LEVEL CFD PROCESS SIMULATION FOR DEVELOPMENT OF FLUIDISED BED BIOMASS GASIFICATION

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ABSTRACT

The integration of simulation tools into development processes of reacting CFBs creates process understanding and optimisation opportunities at very early stages and thus helps to avoid costly wrong decisions. It can significantly reduce time requirements while increasing the quality of the resulting process.

INTRODUCTION

The use of software-systems in complex development processes is well-established in automotive and aircraft industry (1, 2). Transferring such methods and tools to the design of a circulating fluidised bed creates benefit, as overall development time can be reduced considerably while process understanding and degree of optimisation is increased. Reacting CFBs are complex processes that comprise multi-scale problems with regard to time, dimension and physical phenomena. The complete process with all required components can easily reach a size of several meters but still contains functional relevant structures down to a few millimeters in size e.g. the fluidisation nozzles. Time scales for CFBs range between seconds for pressure or velocity changes and several hours for reaching stationary temperatures, mass content or particle size distribution in the complete plant. The strong dependencies between separate components of the process dictate a concerted development. Design decisions have to be tested at very early stages and within the complete process even though not all of the details are fixed yet. The aims of the here shown staged development method are:

- definition of process parameters and basic dimensions at the beginning of a development process
- prompt tests of design decisions by means of numerical simulation
- support of detail engineering and prevention of long and costly corrections at later stages
- compilation of simulation tools for planning of experiments pilot-scale facilities
- fast interpretation of in-operation phenomena

In order to minimise response times and numerical effort, the complexity of the simulation matches the stage of development and the problem being addressed.

NUMERICAL SIMULATION IN FLUIDISED BEDS AND DENSE PARTICLE FLOWS

The major challenges to be met in fluidised bed simulation are the couplings between gaseous and particle phase kinematics with simultaneous particle combustion. The Multiphase-Particle-In-Cell (MP-PIC) method overcomes those shortcomings by a computationally efficient bi-directional coupling between the discrete motion of Lagrangian particles and the continuous gas phase for which the Navier-Stokes equations are solved (3). The MP-PIC method discretises the physical particle space by numerical 'parcels', thus enabling full technical scale fluidised bed combustion in economic time scales. The simulation is strictly transient, thus accounting for the inherently fluctuating character of flows with high solid volume fractions (4).

In the lower part of a CFB where the flow is dense with local solid volume fractions > 10%, the two-phase flow is governed by the particle-particle interactions. Typically the fuel is injected into this region, so the proper computation of solids mixing and jet penetration is crucial for the prediction of process characteristics. The MP-PIC method considers particle interactions by integrating the discrete particle properties in each computational cell, hence forming a particle stress tensor for which a transport equation is computed within the Eulerian cell frame. The result of this solution is then mapped back onto the respective position of each single particle. This hybrid particle interaction model then solves the particle equation of motion

$$a_p = D_p \left(u_f - u_p \right) - \frac{\nabla p}{\rho_p} + g - \frac{1}{\Theta_p \rho_p} \nabla \tau_p$$

A characteristic feature of the MP-PIC method is that particles displace the surrounding continuous phase. As a consequence, the computational domain for the Eulerian phase is a highly complex transient 3-dimensional space. This method enables the realistic representation of all particle regimes from dilute to dense flow with typical large scale fluctuations and cluster and streak formation. In the present work, the MP-PIC method is used within the commercial software package Barracuda VR.

For reacting flows, continuous phase momentum transport equations and particle motion are coupled with scalar equations for energy and gas phase species (N_2, H_2O, CO, CO_2, CH_4, …). The set of equations is completed by closure terms for homogeneous and heterogeneous reactions. The respective reaction rates are computed at each location and time step. A full description of the kinematic and chemical model is given in (5).

The resulting sequences of instantaneous variables provide the user with a deep insight into the structure of complex dense particle flows. Time- and space-averaging of instantaneous values enables quantitative studies and form the base for comparison with measurements. Nevertheless, all information about variable fluctuations is preserved.

MULTI-SCALE-SIMULATION METHOD

A major challenge for fluidised bed simulation is the existence of multi-scale time phenomena. Pressure and velocity fluctuations occur in the range of seconds or below, while solids amount and particle size distribution in the complete CFB loop take hours or days to develop a quasi-stationary state. Analysis of short-term phenomena often requires knowledge of data from long-term evolution that is not available from the initial engineering approach. The correct prediction of local temperatures and concentrations as well as the fluidisation and solid carry-over requires exact boundary conditions for mass flow, temperature and char content of the recycled bed material which are not known. Here, data from a simple process model computed to steady state conditions gives a first and fast feedback on the design and serves as a good initialisation for a more detailed simulation.

Starting from a best practice engineering approach of a given process concept and parameters a rough initial design is defined. This design is evaluated in a virtual testing environment. The level of detail of the simulation in the testing environment starts low and is increased gradually as the initial design is refined. At each stage the latest improvements are evaluated numerically, simulation results are used to confirm or revise and improve a design decision. The level of detail of the simulations for each stage is kept as low as possible in order to keep the numerical effort and the response time low. Results are furthermore used to verify previous results from less detailed simulations and to provide more detailed insight of the overall process and thus better boundary conditions for more detailed simulations to follow later on.

The process model constitutes the simplest description of the plant, already featuring the correct gas solid mass flows as well as the complete chemical reaction system. The CFB's basic geometry is simplified, conserving the real

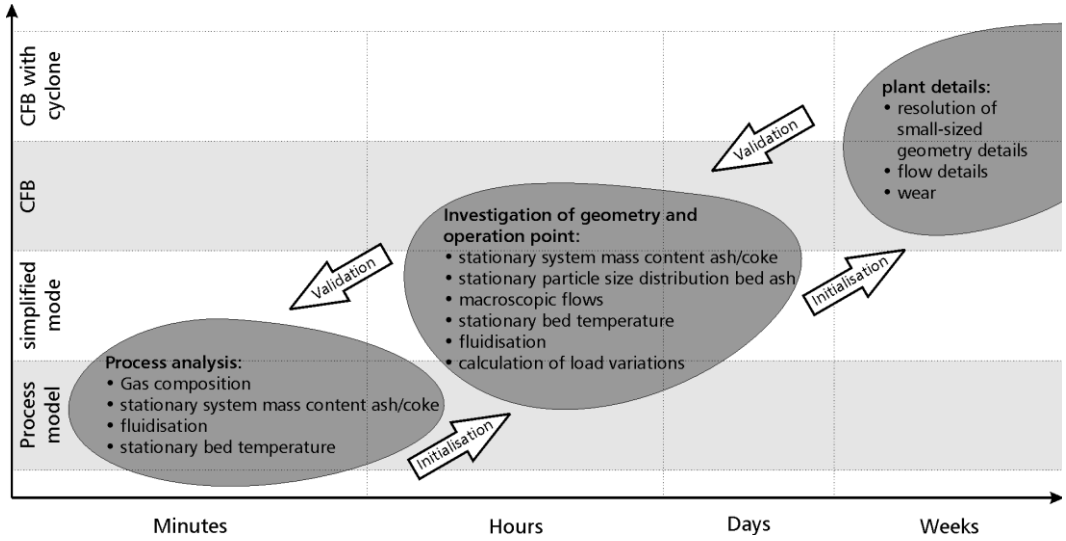

Figure 1: Flow of information with the multi-level simulation concept, Comparison of level of detail and simulation time and effort

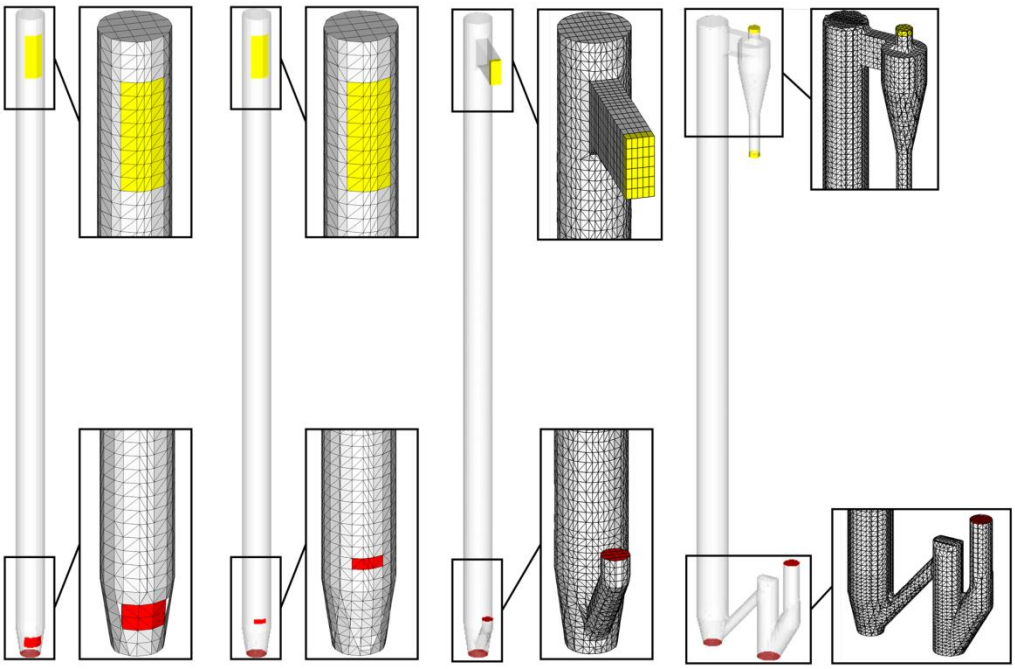

Figure 2: Representation of employed geometry and the computational grid in the process model (leftmost), the simplified model (left-hand side), the detailed model (right-hand side) and the complete model (rightmost)

geometry's ratios of volume flows to cross-sectional areas and allowing first conclusions concerning fluid behavior to be drawn. Unknown boundary and initial conditions that can only be met by assumptions at the beginning of the simulation form the center of interest. The process model's short computation time enables calculations to run up to stationary states under the given boundary conditions and assumptions and thus renders pre-estimations concerning the heat balance, the fuel and ash balance as well as the resulting particle size distribution possible. Especially the resulting temperatures and the system's fuel mass content and carry-over are of major importance since these parameters determine the result's quality significantly due to their considerable feedback (s. Figure 3).

Process models allow a rapid investigation of the process feedback to macroscopic boundary condition and geometry changes and enable estimations of their efficiency concerning the specific issue.

Basically constituting a sophistication of the process model, the simplified fluidised bed model is made up of about ten times more cells and numerical particles. The simplified model already provides first insights into flow structures in the fluidised beds still omitting small-sized geometry details. By these means, the model does not give an exact representation of the gas inlet's momentum and direction, unless the gas enters the system normal to the system's wall.

In consequence, the simplified model helps to improve and validate the estimations derived from the process model. The simplified model's boundary and initial conditions benefit from the process model's results, especially

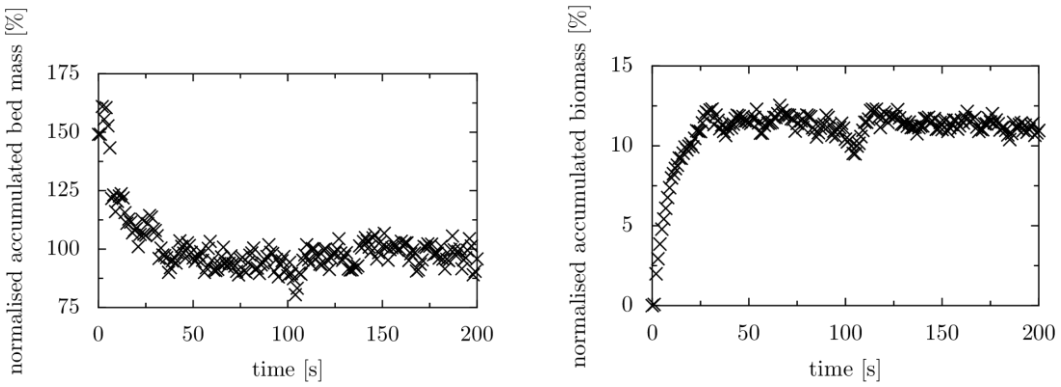

Figure 3: Normalised evolution of circulating bed material (left-hand side) and coke (right-hand side) mass content within the system over simulation time in the process model

stationary particle mass contents and temperatures, and by this way speed up the calculation time required to achieve significant and stationary results.

The detailed model is yet again about ten times larger than the simplified model. It involves a higher local resolution and precise inlet boundary conditions including momentum and direction as well as small fluid motion-relevant geometry details. By this, the model enables the investigation of the local flow structures and the influence of comparatively small geometry modifications. In addition to the investigation of the mentioned parameters, the calculation of local gas and particle velocities enables significant investigations of a plant's wear. As described in Table 1, amounting to about six weeks for 60 seconds of simulated time, the calculation time for a simulation at this level of detail for an entire plant is rather high. Starting off with the initial conditions chosen at the beginning for the process model, the computational time for a simulation at this level of detail including transient starting effects and the computation of a sufficiently large time span in order to be able to significantly average non-stationary results is about 30 days. Implementing the ash and coke mass content as well as the resulting bed temperatures attained by means of the process model and the simplified model, the initial transient effects are shortened and the total computational time is reduced by 30-50%.

	Process Model	Simplified Model	Detailed Model
Computational Cells	2.300	18.000	250.000
Numerical Parcels	17.500	150.000	3.750.000
Computational time for 60 seconds (Real time)	15 minutes	9 hours	5 weeks

Table 1: Comparison of the multi-level simulation concept's different levels with regard to resolution and computational time (on a single core processor). The complete boiler contains around 300 kg of solids with roughly 10^{12} particles.

APPLICATION OF MULTI-SCALE-SIMULATION METHOD IN A DESIGN PROCESS

The shown method is used to dimension a gasifier to produce high quality synthesis gas from biomass for industrial purposes. Apart from the projected plant size to be equivalent to a combustion with a thermal load in the order of 2 MW (a typical pilot scale), the size and geometry is undefined. In order to produce a high calorific gas, the heat for the gasification process is to be provided by an external source and transported into the reactor by means of preheated, recirculated bed material (e.g. sand).

From this very basic specification a plant concept is derived which consists of a CFB to provide the necessary heat and mass transfer during the gasification and to ensure a high carry-over of bed material in order to be able to transport the gasification heat into the reactor. Subsequently the plant concept is transferred into a basic dimensioning of the CFB reactor which is evaluated in a simulation at process model and simplified model level.

In the process model the engineering approach is tested and key parameters like amount of fluidisation, solid matter content and reactor dimensions are varied. Short simulation times allow for a high number of parameter variations on this level of detail providing a comprehensive overview of the effect and range of influencing variables (s. Figure 4 for examples).

Promising settings are re-evaluated at the next level of detail in the simplified model. At this stage the higher computational cost implicates a higher exactness with respect to physical behavior while still offering the opportunity for a substantial amount of variation simulations. Thus the global properties and dimensions, e.g. gas and solid matter mass flows and reactor diameter, of the process can be decided at this point of the design process.

Now geometric details like shape and position of the ash reinjection, the fluidisation grid or the ash drain are included and tested on the level of the detailed model. Again the simulation acts as a verification for the results of the less detailed models used before. Apart from this the influence of geometric

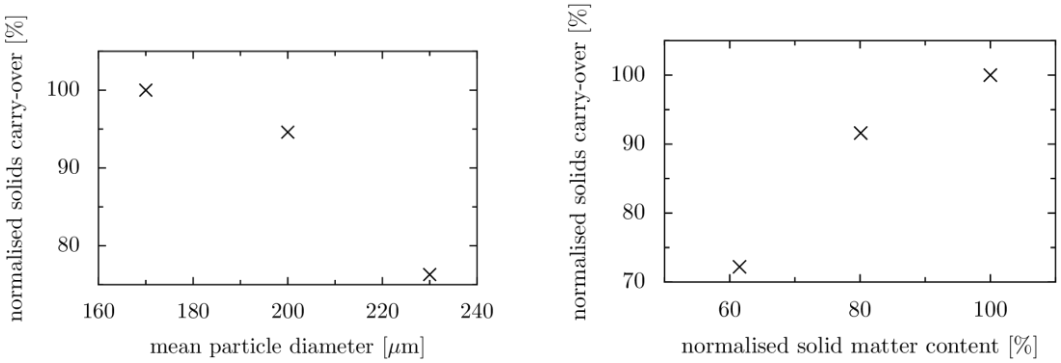

Figure 4: Showcase plots of the effect of influencing variables on solids carry-over: solids carry-over against mean particle diameter of bed material (left-hand side) and against amount of solids contained in the riser of the CFB (right-hand side).

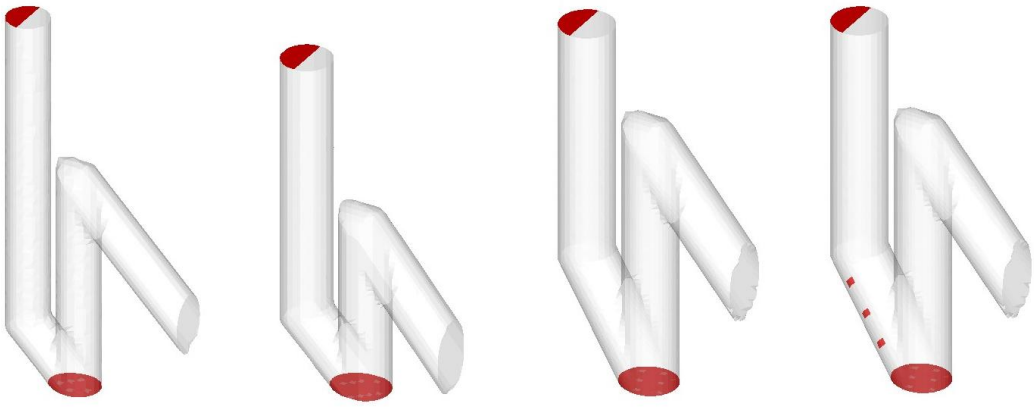

Figure 5: Evolution of basic siphon design from first design (leftmost) over a version with increased diameter (left-center), a version with increased slope angle (right-center) to version ready for detail optimisation (right).

details, the interaction between components like ash chute and fluidisation grid and their influence on the fluidised bed or the intermixture of reinjected bed material and biomass can be evaluated at a high local and temporal scale.

With the basic concept in place, the details of auxiliary but nevertheless important components of the process like cyclones or the siphon have to be considered. Following the same staged approach as before the starting point is a rough best practice engineering approach followed up by an incremental increase in detail.

The specification requires the siphon to be able to transport the solid carry-over from the CFB at the design point while it has to seal the pressure difference between the lower end of the CFB and the cyclone. At the same time the solid mass in the siphon should be low and there should be no resting particles.

The initial design consists of a simple U-pipe with fluidisation below the riser (Figure 5). The drop tube ends in a slope to transport the solid material towards the fluidisation grid. To keep the volume of the siphon low a small pipe diameter is selected. The numerical evaluation in the simplified model shows too little solid matter throughput, but apart from that the simulation gives valuable information

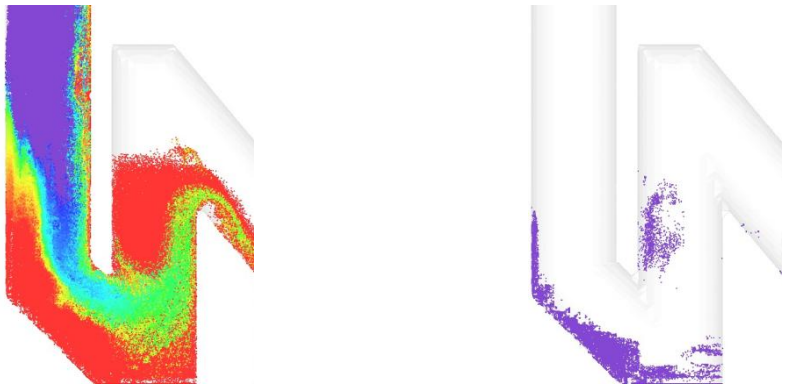

Figure 6: Sand particles coloured by residence time (left-hand side), blue particles have a short, red particles a long residence time. Particles selected by their momentary velocity, only particles slower than 1 cm/s are shown (right-hand side).

about the functioning and thus about the causation. As can be expected an increase of the siphon diameter helps in increasing the throughput but at the same time it increases the volume. From the simulation results a bottleneck within the siphon can be identified as there are resting particles on the slope blocking parts of the cross-section of the pipe impeding particle transport (Figure *6*). Based on this insight the slope angle is increased and a few small loosening nozzles are placed. With these changes in place the design meets the specification and can be further refined in detailed simulations.

The above shown steps of the development process of the siphon were done in about two weeks with around 20 Variations in geometry and boundary conditions. Implementing the shown design methodology the time necessary from the definition of a basic concept of the siphon up to an engineering drawing is roughly 4 months only.

CONCLUSION

Integrating software-systems into complex development processes is a well-established concept in other fields and it shows good results for the development of complex processes like CFBs. The multi-scale simulation method presented in this paper is capable of supporting conventional engineering approaches at each level of detail of the design process. Due to its variable complexity, which is matched to the problem at hand, it gives fast results, the opportunity to check decisions and to optimise each step properly. The overall development process can be speed up and significantly improved by the increased process insight which is created at very early stages long before a mechanical implementation can be build and tested.

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