Simulation of the particle flow in a twin-screw mixing reactor for fast pyrolysis of the biomass residues

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Motivation

The twin-screw mixing reactor, used for fast pyrolysis of lignocellulosic material at the PYTHON plant, proves to be a robust and effective reactor for fast pyrolysis of biomass. Regardless the positive operation experience, there is a little systematic knowledge about design criteria for this kind of reactor. At this point, a numerical approach to simulate the particle behavior (Discrete Element Model) and the fluid behavior (Computational Fluid Dynamics) comes in hand.

Computational Fluid Dynamics (CFD)

Introduction

Computational Fluid Dynamics (CFD) is a commonly used technology for the simulation of fluid dynamics. One of the many software packages at this field is the open source program OpenFoam®. This software package is known for its exceptional solvers and boundary conditions adaptability.

Previous work

Fluid flow in an empty reactor

U Magnitude (m/s)
0   0.5   1   1.5   2   2.36
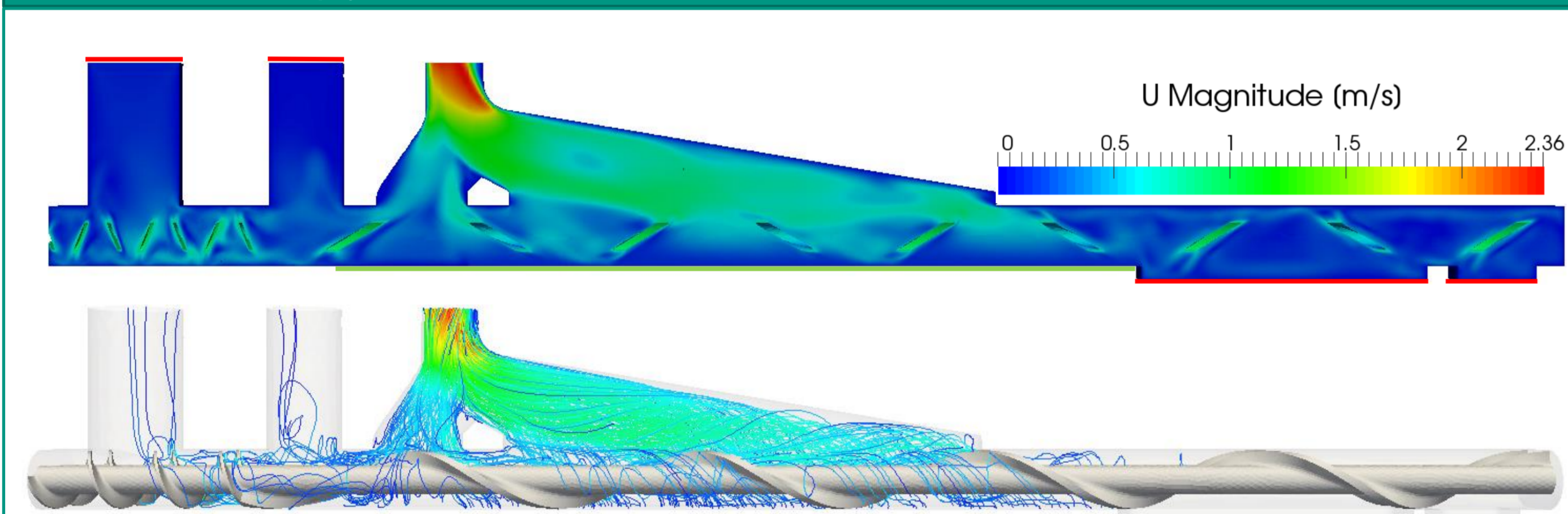
The simulation was done, at fixed state of the reactor. For this simulation, nitrogen was injected at the inlet points marked with red, at the heat carrier inlet and outlet as well as the biomass inlet. Pyrolysis gas was created with a constant velocity, at the with green marked reaction area. The lower picture shows a stream-tracer, which follows the fluid movement back, starting from the pyrolysis gas outlet.

Conclusions

- It is possible to simulate the fluid phase of a complex geometry using OpenFoam®.
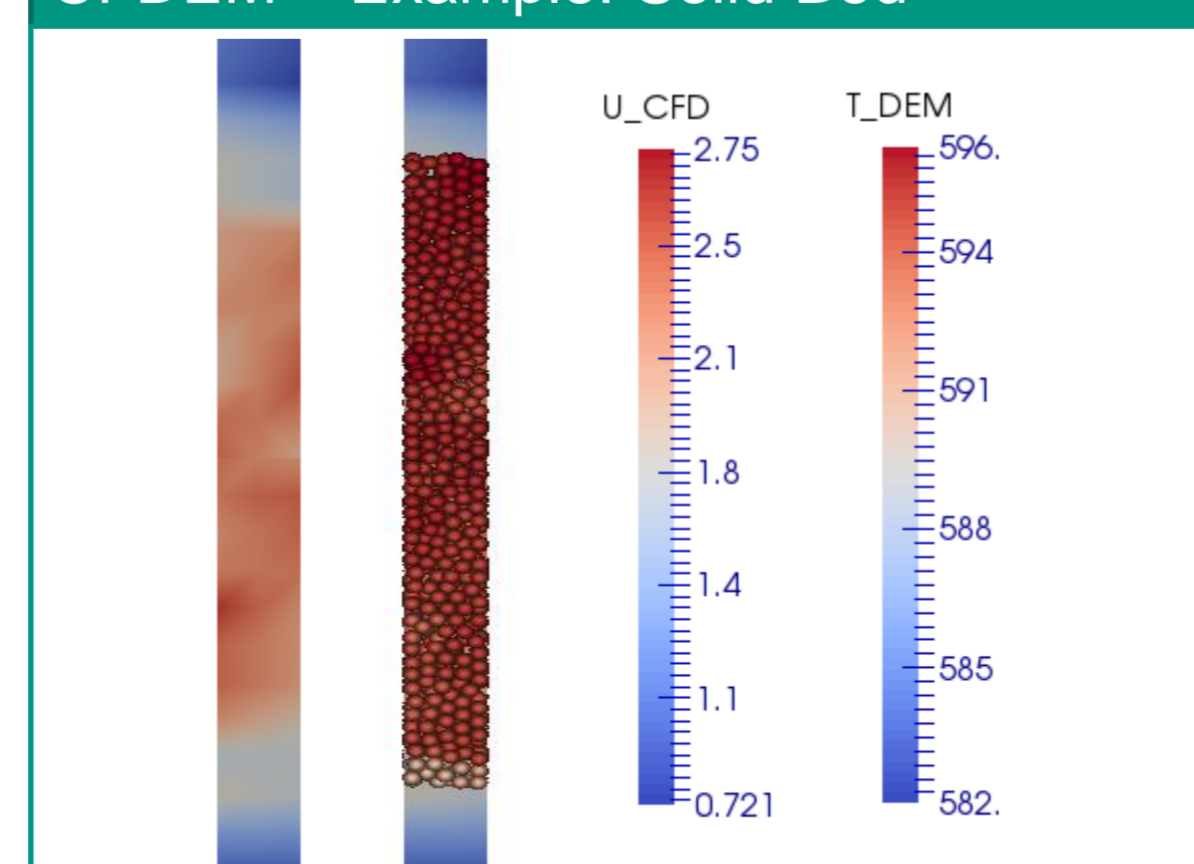
Ongoing activities

- Using immersed boundary methods, the movement of the twin-screws will be implemented.
- Implementation of a thermodynamic solver for improving the accuracy of the results.
- Determining the pyrolysis conversion rate of biomass.

CFDEM - Approach

The open source program LIGGGHTS® was developed with the perspective to couple it with OpenFoam®, which means having both advantages of DEM and CFD. This can be done with the package CFDEM®-Coupling, which is developed by DCS-Computing.
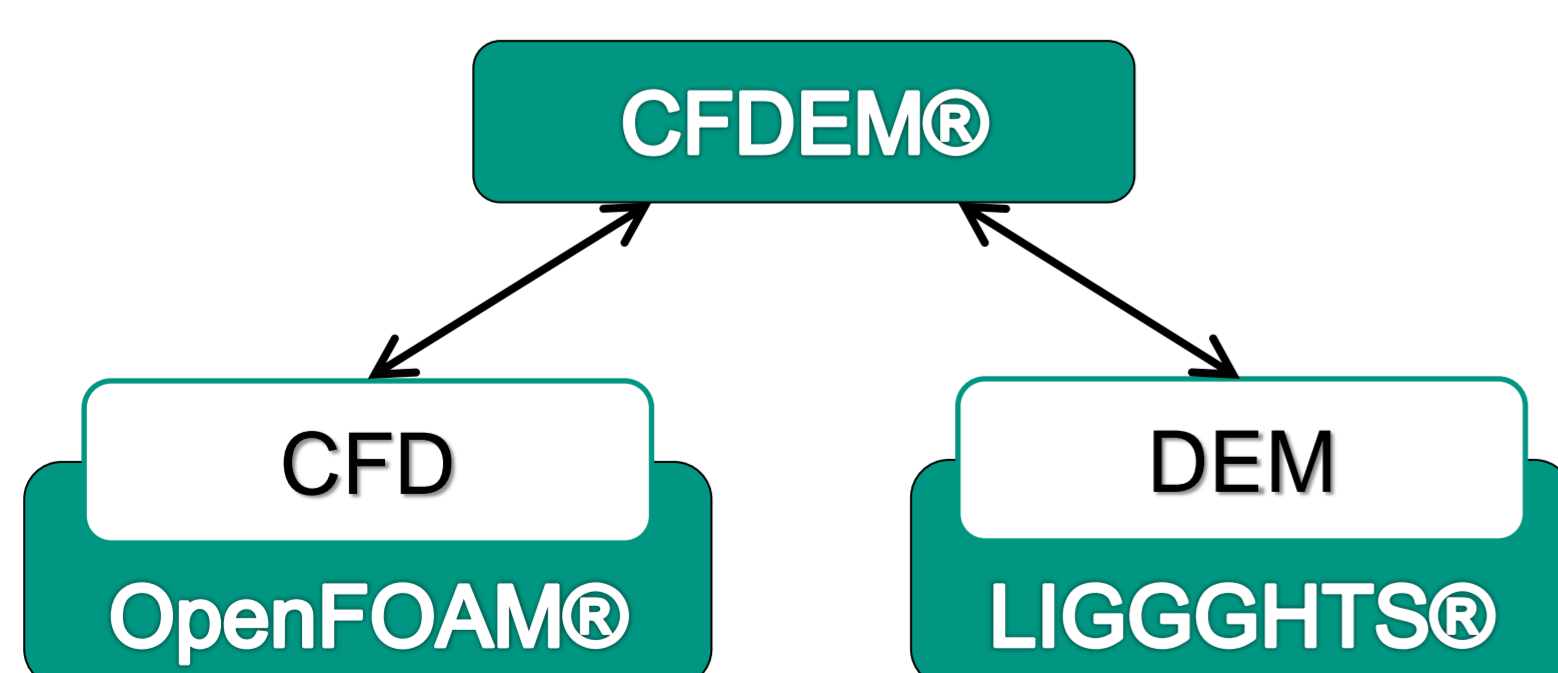
CFDEM – Example: Solid Bed

U_CFD   T_DEM

Using CFDEM®, it is possible to simulate the influence of a particle bed to the fluid.

Ongoing activities

- Verification of the CFDEM-Simulation.
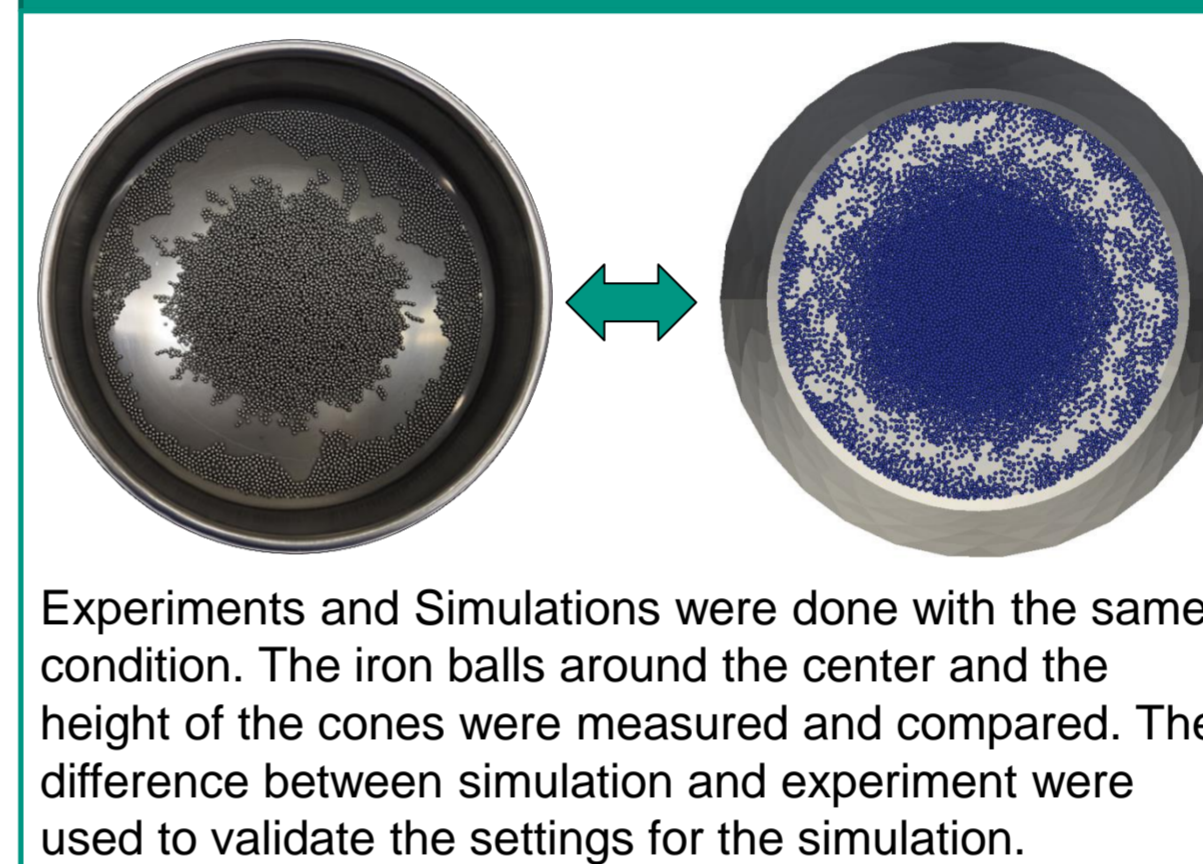- Implementing the CFDEM® approach in the immersed boundary – multiphase solver.

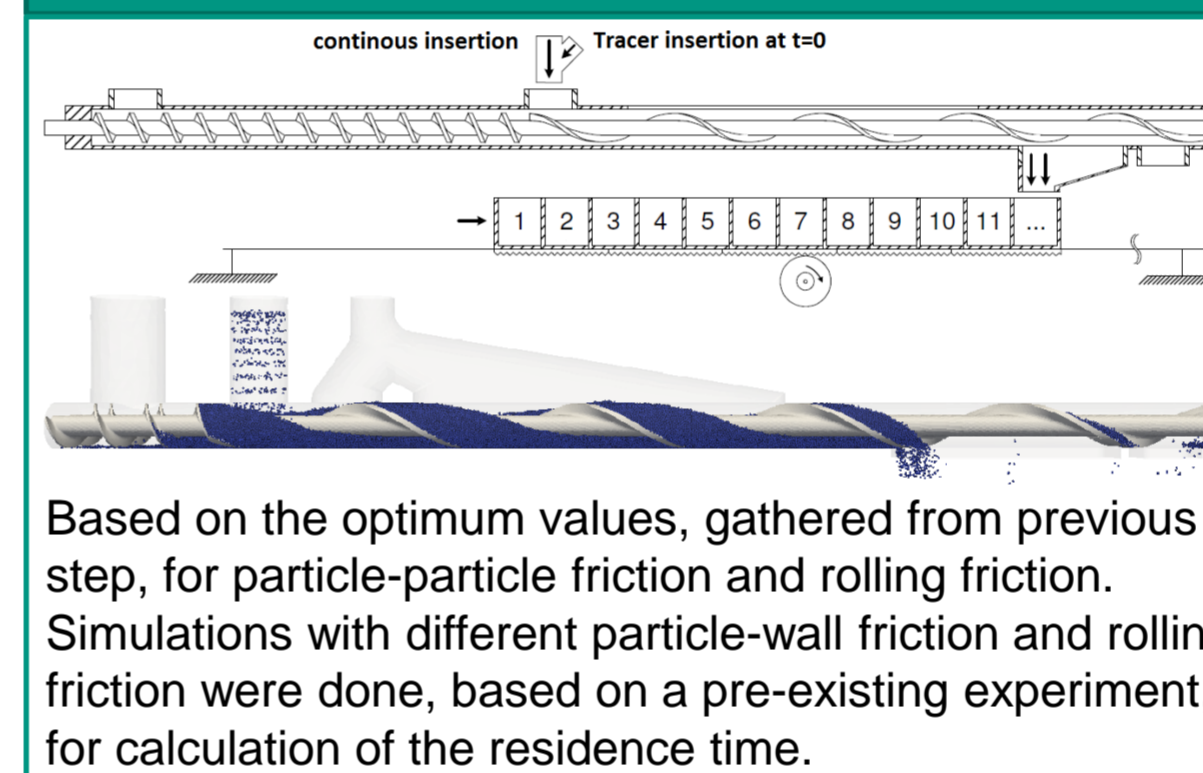## Discrete Element Model (DEM)

Introduction

DEM is a method which uses Newton´s mechanical laws to simulate the solid particle kinetic of a great number of spherical particles. The program which is used for DEM-Simulations is LIGGGHTS®-Public, an open source tool developed by DCS®-Computing.
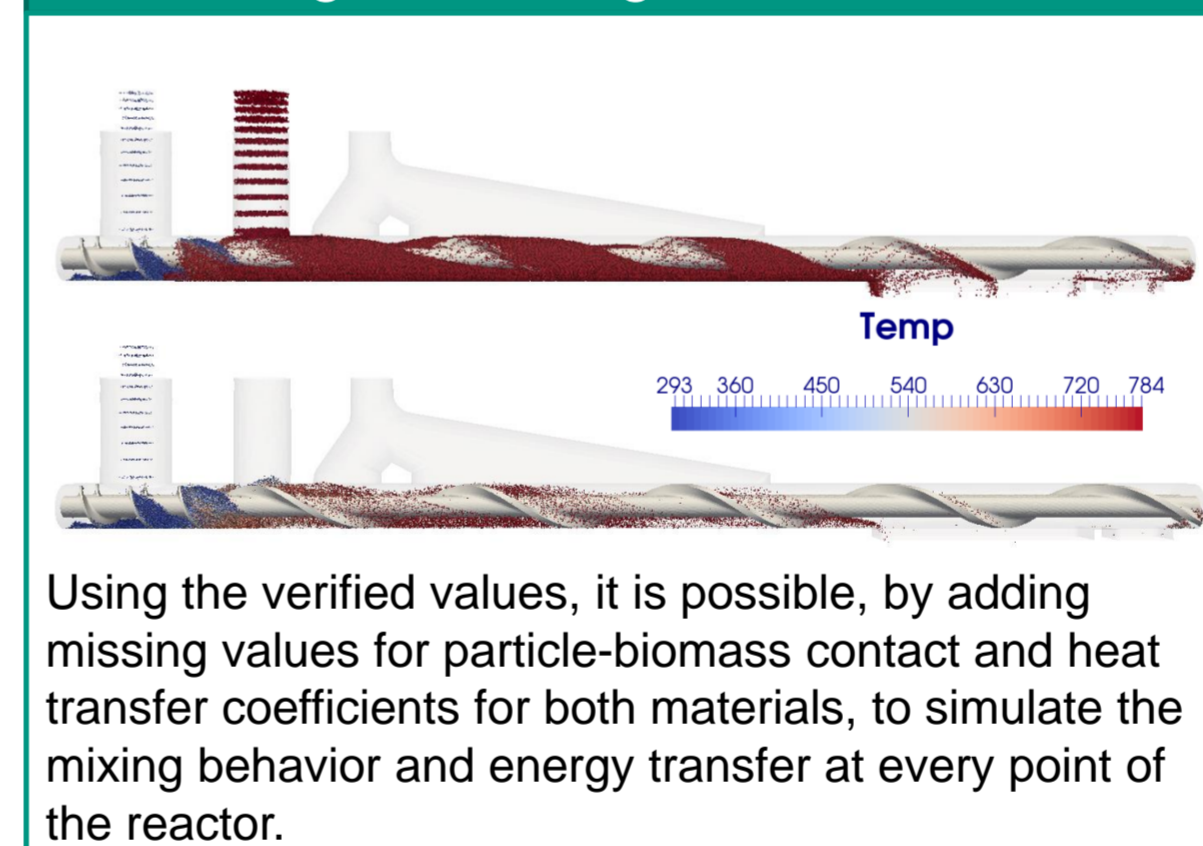
Previous work

Determination of values

Influence of friction and rolling friction on steel spheres

Experiments and Simulations were done with the same condition. The iron balls around the center and the height of the cones were measured and compared. The difference between simulation and experiment were used to validate the settings for the simulation.

Verification of values

		4 Hz	3 Hz	2 Hz
Experimental [1]		9,6 s	12,4 s	17,8 s
Simulated	p-w rf=0,2	9,3 s	13,6 s	18,8 s
	p-w rf=0,17	8,5 s	12,7 s	17,8 s
	p-w rf=0,15	8,1 s	12,3 s	17,5 s
	p-w rf=0,12	7,3 s	11,2 s	16,5 s

Table: residence time with different operating conditions

Based on the optimum values, gathered from previous step, for particle-particle friction and rolling friction. Simulations with different particle-wall friction and rolling friction were done, based on a pre-existing experiment, for calculation of the residence time.

Simulating the mixing behavior

Temp
293 360 450 540 630 720 784

Using the verified values, it is possible, by adding missing values for particle-biomass contact and heat transfer coefficients for both materials, to simulate the mixing behavior and energy transfer at every point of the reactor.

Mixing quality in the twin screw reactor

Temperature of the biomass particles
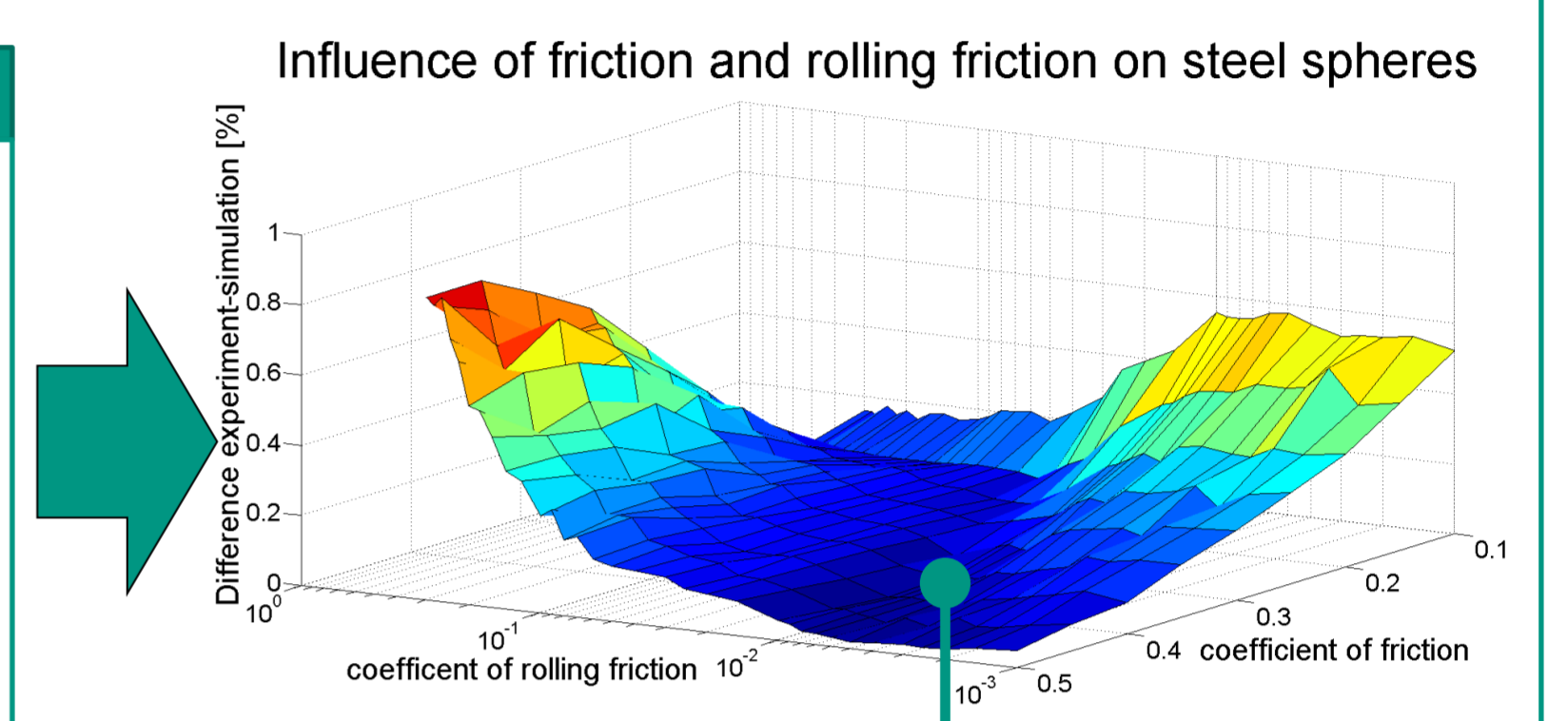
Temperature gradient of the biomass particles

Conclusions

- It is possible to simulate the mixing behavior with high accuracy.
- The residence time is strongly dependent on particle-particle, particle-wall friction and rolling friction.
- The simulation shows some dead zones, which indicates that there is still a potential to improve the reactor design.
- DEM simulation can be used for validating a new reactor design and screw geometries.

Ongoing activities

- Improvement of simulation quality by the determination of biomass-related friction as well as rolling friction.
- Improvement of the LIGGGHTS® results by using rigid bodies for simulating non spherical particles.

[1] **Kornmayer, Christoph**: (2009) *Verfahrenstechnische Untersuchungen zur Schnellpyrolyse von Lignocellulose im Doppelschnecken-Mischreaktor*: Dissertation: S.51

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