OPTIMISATION OF THE WET FLUE GAS CLEANING PROCESS THROUGH MODELLING THE USE OF DROPLET INTERACTIONS IN OVERLAPPING SPRAYS

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Abstract
In most large coal-fired power plants the absorption of flue gas with a limestone suspension is an important unit operation for keeping gaseous emissions within the specified limits. The flue gas proceeds upwards through a series of spray headers that introduce an uniform liquid flux of droplets of the limestone suspension. These droplets resist the gas flow and provide a large mass transfer surface area required for the SO_2 removal process. During the spray overlapping the collision of the droplets may lead to a coagulation or a separation process depending on certain collision parameters such as surface tension, impact velocity and collision geometry. In the wet flue gas cleaning process the droplet collision results usually in a break-up of the droplets, therefore it is an effective mechanism to increase the specific mass transfer area. Experimental investigations confirm the speculation that droplet collision have a significant influence on the droplet size [1] and the absorption in a flue gas scrubber [2,7]. Therefore, it is important to take droplet collisions into account for simulation of this process, which is the main focus of this paper.
In this paper the collision model of Dohmann [2], experimental results and CFD-simulation are used to predict the change of the specific surface and droplet size refinement. In addition, it enables to get an enhanced nozzle alignment in consideration of the effect of droplet collisions.

The simulation program

For calculating the available mass transfer area for the desulphurization process in wet scrubbers, a stand-alone simulation program with a detailed model for the disperse phase and the interactions between the disperse and the gas phase is used. The software consists of a Lagrange-solver for the disperse phase and a Navier-Stokes-Solver for the continuous phase in a separate modul. The program with the name sIMPACT (simulation of particle collisions in turbulent flow) was developed in the programming environment Borland C++. Figure 1 illustrates the logic program architecture and the applied libraries.

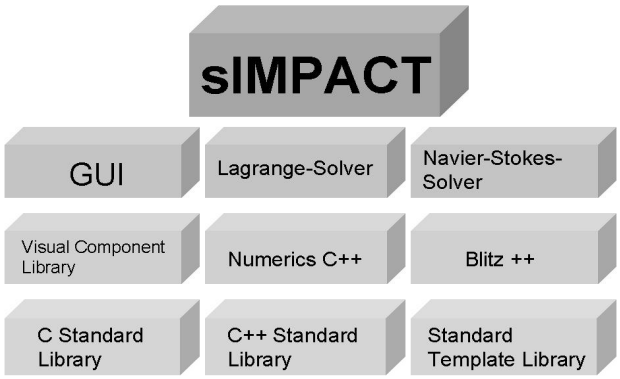

Figure 1: program architecture of sIMPACT, a stand-alone software

The flow field is discretizised in a three-dimensional orthogonal and equidistant grid by means of finite differences. The discretization of scalars and velocity compounds is made by a displaced grid (Figure 2), whereas the pressure and turbulence values are discretizised in the center of a cell and the velocity component on the cell surface.

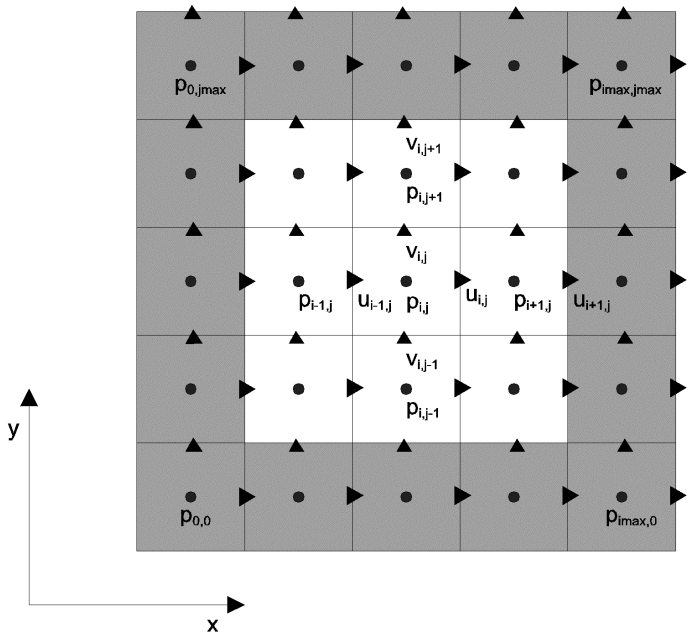

Figure 2: displaced grid (2-dimensional, with margin cells)

The solver is designed as an unsteady solver in principle and uses pseudo-time-stepping to calculate steady results, whereas the time-steps are used for external iteration. The particle tracing is simultaneous. For the solution of the Navier-Stokes-equations, pressure and velocity are degenerated and initially a preliminary velocity field is calculated out of the convection and diffusion terms. Afterwards, a system of equations for the pressure field will be established, whereas the velocity is completely on one side. Thus, the size of the system to solve is reduced. After the calculation of the pressure field, a pressure correction will be added to the preliminary velocity field. Furthermore, the turbulence values will be calculated again. Hence, a timestep is closed and the solver starts the next step again with he calculation of the convection and diffusion field. For the calculation of the turbulence, the standard k/ε-modell (Launder and Spalding) as well as the standard k/ω-modell and the enhanced Wilcox ’93-modell [8] are implemented. For the storage of the variable fields and for a few operations of the multigrid-solver, the free available Blitz++ library is used, wherein template based vector and matrix classes are defined [6]. In case of the solution problem for a system of equations, a C++ developed program can achieve the same performance as a FORTRAN-developed program [6]. The implemented Lagrange-solver can undertake a simultanous calculation as well as a successive trajectory calculation. It turned out that the overall needed calculation time for a simultanous simulation is less than a successive simulation. The need of working memory is slight enough to calculate an adequate number of droplets simultanously.

In the observed flow field, the particle concentration is localy different. Quite close to the nozzles, the particle concentration is very high, other parts have less particle concentration. For an optimization of the dissolution of the grid without wasting working memory and performance, an adaptive mesh refining of the grid is implemented. As soon as a cell contains a maximum number of particles, the cell will be devided into eight smaller cells, each with half edge length. The adaptive mesh refining happens recursive until a certain minimal edge length is achieved. An adaption in areas with high concentration of the disperse phase takes place automatically.

The simulation model

Several attempts of modelling single droplet collisions under certain conditions may lead to accurate results [3-5]. These models need intensive computation, because they describe the collision in detail with an oscillating droplet surface etc.. However, this intensive computation is not possible for our problem due to the high droplet quantity in the flue gas scrubber. Therefore, we perform further experimental investigations whose results are applied to a model that effects a statistic expectation for the disperse phase. The collision model of Dohmann [2] is suitable for calculating the effect of droplet collision on the droplet size using the Monte-Carlo simulation. It is used to make predictions on the change of the specific surface out of statistic values such as droplet mean diameter, mean velocity and mean concentration.

The empirical model assumes that one part of a mono-disperse spray crosses another spray without interaction and the other part effects collisions and break-ups which leads to a droplet size refinement.
Droplet collisions can be described with three dimensionless numbers, the collision Weber number Eq. (1), the diameter ratio Eq. (2) and the impact parameter Eq. (3):

$$We = \frac{\rho_p d_s u_{rel}^2}{\sigma_p} \tag{1}$$

$$\Delta = \frac{d_s}{d_l} \tag{2}$$

$$B = \frac{2b}{d_l + d_s} \tag{3}$$

The impact parameter is a geometric condition for collision and gets the value of $0{,}5 \cdot \sqrt{2}$ in case of a statistic mean value estimation. The collision Reynolds number Eq. (4) has a slight and negligible influence and is left out in the model.

$$Re = \frac{\rho_p d_l u_{rel}}{\mu_p} \tag{4}$$

The break-up coefficient μ is a value that describes the splitting of a droplet into several fragments; it can be derived from experimental data. As a result the break-up coefficient may be described only as a function of the mean collision Weber number and the mean diameter ratio

$\mu = \mu(\overline{We}, \overline{\Delta})$.

The relationship between the collision Weber number and the diameter ratio can be ascertained in experiments with overlapping sprays (Figure 3).

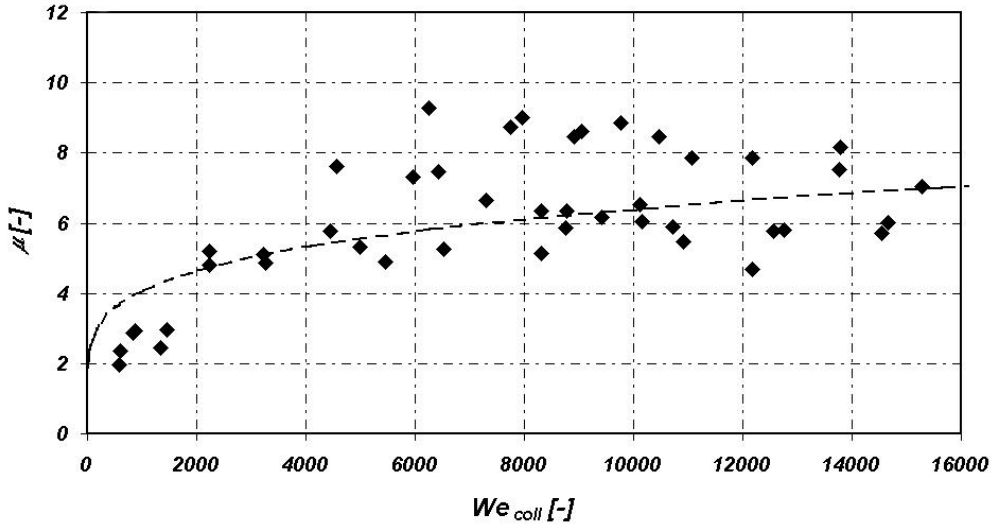

Figure 3. The break-up coefficient for Δ =1 vs. collision Weber number

The following equation Eq. (5) fulfils all conditions for μ for uniform droplets as well as for the collision of nonuniform droplets:

$$\mu(We, \Delta) = \left(1 + \Delta^3\right)^{-\frac{1}{3}} + C_1 \cdot \Delta^{C_2} \cdot We^{C_3} \tag{5}$$

Common constants are $C_1 = 0.66$, $C_2 = 0.23$ and $C_3 = 5.17$. The adaptation of this equation for the collision of nonuniform droplets is received through matching the constants with the least-squares method.

Accomplishment of experiments

In the experiments the spray overlapping of two hollow cone nozzles was approximated with two flat jet nozzles. One single flat jet (aperture angle 20°) corresponds to a 1/18-segment of a ring area of a hollow-cone jet. The droplet size distribution for different experimental conditions was measured by means of particle dynamics analyser (PDA). The experiments were performed with water. According to Wieltsch et al. [3] there is

no difference between water and limestone suspension regarding the measured droplet size distribution and droplet velocity distribution.

Results

Two typical nozzle alignments of two hollow cone nozzles were calculated and are exemplarily presented here to visualize the effect of droplet collision. These alignments exist in a real flue gas scrubber. The fluid system consists of air at 60°C for the continuous phase and water at 60°C for the disperse phase for calculation. The following simplifications are assumed:

- the calculation was isothermal and incompressible
- the quantity of physical droplets increases after collision, in the calculation the quantity of calculated droplets remains the same

Our simulations enable the examination of the nozzle alignment to each other and the influence of droplet collision on the available mass transfer area in detail. This is why a single nozzle and two alignments with two nozzles with overlapping spray cones were simulated. The different alignments of two nozzles were calculated twice, first without droplet collision and subsequently, a droplet collision including.

Tab. 1 gives an overview of the simulation data and the nozzle specification for the calculation of the single nozzle.

Table 1. Simulation and nozzle data

nozzle type	hollow cone	grid: number of cells	30000
horizontal nozzle distance	1220 mm	calculated area	3 x 3 x 3 m
vertical nozzle distance	1500 mm	boundary condition	no slip
spray angle	120°	turbulence model	k-ω (Wilcox ’93)
volume flow per nozzle	18 l/min	discretization scheme	Partial-Donor-Cell
droplet velocity	14 m/s	time step	0.001
mean droplet diameter	1600 µm	maximum number of calculated droplets	150000
gas velocity	0 m/s	total number of simulated droplets	730000
nozzle position [m] X x Y x Z	1.5 x 1.5 x 1.5		

All calculations were carried out in an orthogonal grid. The distance between the nozzle and the edge of the calculated area is about 1 m.

Two neighbouring nozzles on the same level

In the following calculated cases the simulation parameters of Tab. 2 were used. We assume the free slip boundary condition for the continuous phase. The distance between the nozzles is 1220 mm, which is a common distance on one level, the nozzles are arranged in an equilateral triangle. Quite close to the wall the nozzles have smaller distances. In this calculated example the distance is 1220 mm. Tab. 2 displays the simulation data for the calculation.

Table 2**.** Simulation data for two nozzles on the same level

calculated area	3.22 x 2 x 3 m			
gas velocity	5 m/s			
grid cells	30 000			
total number of simulated droplets	3100000			
maximum number of simulated droplets	2500000			
nozzle position [m]		X	Y	Z
	nozzle 1	1	1	1.5
	nozzle 2	2.2	1	1.5

Figure 4 shows clearly an increase of the droplet concentration after the spray overlapping if the droplet collision is taken into account. This effect is stronger in the overlapping of the lower spray cones, which are in counter flow to the gas stream, than in the overlapping of the upper spray cones, which are in current flow to the gas stream. Obviously the droplets are diverted from the gas stream. Due to the momentum exchange between the colliding droplets, the trajectories of one stream diver in the direction of the other stream. The absolute velocity decreases caused by the energy dissipation of collision.

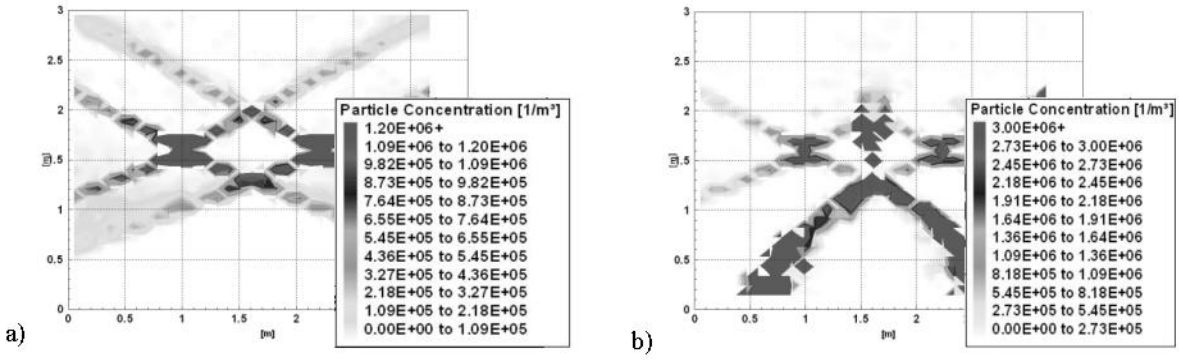

Figure 4. Vertical droplet concentration a) without, b) with droplet collision

Two neighbouring nozzles on different levels

In the following examples the vertical distance between the nozzles is 1500 mm. Tab. 3 gives an overview of the simulation data for the calculation.

Table 3. Simulation data for two nozzles on different levels

calculated area	4 x 4 x 3.5 m			
gas velocity	5 m/s			
grid cells	30000			
total number of simulated droplets	1.500.000			
maximum number of simulated droplets	900.000			
nozzle position [m]		X	Y	Z
	nozzle 1	2.0	2.0	1.0
	nozzle 2	2.0	2.0	2.5

The presentation of the vertical droplet concentration (Figure 4) shows only a small influence of the droplet collision in comparison to the horizontal alignment of the nozzles (Figure 5).

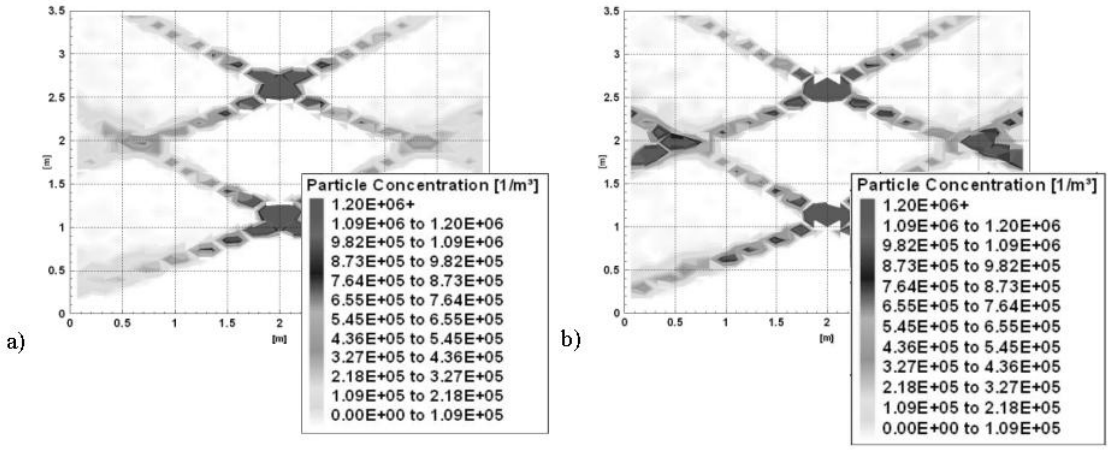

Figure 5. Vertical droplet concentration a) without, b) with droplet collision

Obviously the distance from the nozzle opening to the overlapping area of the spray cone is too large in order to cause an increase of the number of droplets. Whereas the distance between the nozzle opening and the overlapping area is even 700 mm for the horizontal nozzle alignment, the distance for the vertical alignment is 1500 mm.

Summary and Conclusions

The statistic collision model of Dohmann [2] was extended and successfully implemented in a fluid dynamic simulation of different nozzle alignments of a flue gas scrubber. Predictions on the droplet size refinement and the increase of specific surface of the disperse phase are thus possible according to the nozzle alignment. The model is basically suitable for the simulation of spray overlapping.

Simulation results of the available mass transfer area are used to predict the SO_2-reduction in FGD plants. It turned out that in case of old FGD plants, a simple rotation of the lances causes a reduction of SO_2-emission nearly 20%.

Acknowledgements

The development of the model and the experimental investigations are funded by the VGB-Forschungsstiftung (Technical Association of Large Power Plant Operators) and supported by the project department. We express our thanks to the project department of the VGB.

Nomenclature

B	dimensionsless impact parameter
b	distance from the center of the droplet
C	constant
d	sauter mean diameter
u	droplet velocity
Δ	diameter ratio
μ_p	dynamic viscosity of the droplets
μ	break-up coefficient
ρ	specific weight of the droplets
σ	surface tension of the droplets

Subscripts

s	small
l	large
p	particle
i, j	grid point index

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