Customized equipment through flow simulations

Optimization of flue gas purification

Flue gas purification in power plants is an established process. In order to comply with the customer demand for tailor-made systems, Sulzer Innotec makes use of flow simulation. Intensive measurements are performed on test stands to validate the computer models. This procedure helps Sulzer Innotec provide its customers with fast and high-quality consultation on their engineering and on the optimization of their equipment.

In coal-fired power plants and waste incinerators, coal or waste is burned to gain heat and electricity I. Flue gas is produced during the combustion, which, in addition to gaseous nitrogen oxides (NO_x) and sulfur dioxide (SO₂), also contains solid ash particles. In general, flue gas purification consists of the following 3 steps:

Condense

- DeNO_x plant (SCR—selective catalytic reduction)
- Dust deposition
- Desulfurization

Cooling tower

1 Flow diagram of a thermal power plant with flue gas purification equipment.



Fly ash

Flue gas purification

The SCR process is established to remove nitrogen oxides from the flue gas. In this process, the nitrogen oxide elements are reduced to atmospheric nitrogen and water in a honeycomb catalyst by means of gaseous ammonia or an aqueous ammonia solution. Both the gaseous ammonia and the ammonia solution must be fed into the flue gas in a suitable manner and must be homogeneously mixed with the flue gas using mixers. Sulzer Chemtech has solutions available for both steps, i.e., the injection of the additive and the mixing.

Electrical filters are used to remove the dust. In a first step, the dust particles are heavily charged in an electric field. Because the electrical force is perpendicular to the flow direction of the gas, the charged dust particles migrate to the collecting electrode, where they are discharged. At regular intervals, the collecting electrodes are cleaned, and the dust is retained in a collecting hopper.

The process that has mostly been adopted worldwide for desulfurization is lime scrubbing. In this method, gypsum is produced through the addition of lime. This procedure generally takes place in a countercurrent washer, the absorber. Here, the flue gas flows through a column from the bottom to the top. A liquid washing suspension containing lime is sprayed into the column at several levels in countercurrent. The spray trickles downwards, is finely divided, and thereby reacts with the sulfur compounds contained in the flue gas.

Damage due to abrasion

Depending on the operation of the plant, the above steps can also be performed in a different order. If the dust removal takes place after the DeNO_x plant—as in the sequence described here—the proportion of dust in the DeNO_x plant



2 Damage through abrasion on a flange.

will be high. The high dust pollution can significantly reduce the lifetime of the catalyst by abrasion induced by the dust particles.

In order to meet the environmental specifications, the expensive catalyst will have to be replaced more frequently in this case. The other installed elements, such as the ammonia feeder, the static mixer, or even the baffle plates and the channel walls, could also be damaged and even be destroyed in extreme cases [2].

Tailor-made systems thanks to simulations

Sulzer Innotec carries out CFD simulations (computational fluid dynamics) for the design and optimization of $DeNO_x$ plants. The advantage here is that various possible configurations of the internals can be simulated at an early phase of the project. Based on these simulation results, the ammonia feeder, the static mixers, and the other additional equipment—such as the baffles—can be selected in such a way that a tailor-made solution can be offered for every plant.

In this context, tailor-made means that an optimal mix of the ammonia can be determined and a homogeneous flow perpendicularly aligned to the catalyst can be specified, which will minimize the pressure drop for the built-in elements.

Validation of the simulations

The appropriate selection of the simulation domain, the physical model, and the numerical solvers are of great importance to the simulations. Sulzer Innotec has been active in the field of CFD simulations for more than 20 years. A focus of these activities has always been the simulation of flue gas purification plants.

Thanks to the collaboration between Sulzer Chemtech and Sulzer Innotec numerous measurement data are available for the validation of the simulation results. As it is often very difficult to carry out measurements in plants that are in operation, most measurements have been carried out in physical models. In such model tests, the flow conditions can be set up analogously to those in the real plants. Thanks to these extensive measurements, it can be ensured that the appropriate models and simulation methods are available for each problem **3**.

Process in a DeNO_x plant

The variety of influencing factors and models that must be taken into account in the simulation will be explained through the example of a flow simulation of a DeNO_x gas purification plant.

DeNO_x plants can basically be simulated in three different ways that differ with regard to complexity and depth of modeling:

- $DeNO_x \rightarrow gaseous addition$
- $DeNO_x \rightarrow liquid addition (spray)$
- Abrasion through dust particles

Gaseous ammonia addition

The simplest modeling type is the addition of a gaseous ammonia-water mixture (in this case, the ammonia water is evaporated externally) in a dust-free exhaust gas flow. The added ammonia can be treated as a tracer gas. This means that the ammonia has the same material properties and the same hydraulic behavior as the exhaust gas flow. This approach is justified due to the low concentration of ammonia in the exhaust gas in question. The gaseous ammonia is distributed selectively over the cross section with the help of a so-called AIG distributor (ammonia injection grid).

Crucial for high catalyst efficiency, i.e., a high conversion rate and low ammonia slip, is that the local ratio of ammonia to NO_x is as close to the stoichiometric values as possible through the flow. Here, the static mixers from Sulzer Chemtech are of great importance. In addition to providing high-quality mixing of the ammonia into the flue gas over a short distance, they also compensate for local temperature and NO_x peaks.

This is important because the temperature profile and NO_x distribution vary depending on the operating conditions. The static mixers assure a homogeneous NO_x : NH₃ ratio before the catalyst and

3 Validation of the simulation results with measurements from the test stand—on the left, the test stand; on the right, the simulation model (the colors show the velocity: red = high, blue = low).



thus an efficient catalyst operation for a wide load range. This behavior is often achieved with a lower pressure drop than for systems without mixers because a complex ammonia injection system is not required anymore. The main results of the simulation of such a system are the prediction of the pressure drop and the prediction of the mixing quality.

Liquid addition (spray) of aqueous ammonia solution

As gaseous ammonia is poisonous, there is, in densely populated areas, a growing tendency to add an aqueous ammonia solution instead of gaseous ammonia. The aqueous ammonia is thereby atomized in nozzles. The liquid droplets evaporate in the hot flue gas flow and gaseous ammonia is released.

The modeling of this process is much more complex. In addition to the modeling of the pure gas flow, the trajectories of the liquid droplets must also be considered. During their flight, the droplets heat up and evaporate. Suitable models are therefore required to describe the heat transfer to the droplets and to describe the mass transfer from the droplets to the gas. The droplet size distribution, the droplet velocity, and the spray angle of the nozzle are major factors that influence the modeling quality.

Thorough knowledge of the droplet size distribution is important: small droplets have lower momentum and will more likely follow the main flow than larger droplets. They will also evaporate more quickly. If droplets come into contact with a wall, a liquid wall film can be formed, which may lead to problems due to deposition at the wall. Therefore, the aim is to install the nozzles in such a way that all the droplets evaporate before they reach the wall. In addition to the pressure drop and the mixing quality, the droplet trajectories are also of interest in this kind of simulation.

Abrasion through dust particles

Independent of the type of injection addition, the effect of the ash and dust particles on the combustion process of the plant can also be simulated. The main point of interest is to localize where these particles could accumulate and to what extent they could cause damage to the plant through abrasion. In this case, the third phase, the solid particles, also have to be simulated.

An accumulation of particles takes place in regions where the flow velocity of the exhaust gas is low in relation to the descent rate of the particles due to gravity. If the frictional and adhesional forces at the wall are higher than the momentum of the flow, the particles will remain and accumulate at the location they have fallen.

The abrasion depends on the local erosion rate of the particles at the wall. The erosion rate is a function of the particle mass, the speed of the particle, the angle of impact, and the frequency with which a particle impacts a specific location on the wall. Therefore, it is important to know the exact particle size distribution of the dust and to simulate the particle trajectories exactly. For example, an elbow in the channel leads to an increasing concentration of larger particles in the outer part due to higher centrifugal forces. The smaller particles that follow the flow tend to remain in the middle of the flow. Less damage can, therefore, be expected here.

Once the locations that are vulnerable to erosion have been identified with the help of a CFD, there is the possibility of applying a specially-developed thermal-spray coating at these locations, which will massively reduce the rate of erosion [4].

Customer benefits from simulations

By means of flow simulation and thanks to the intensive validation of the tools used, Sulzer Innotec is able to simulate even complex processes in flue gas purification. This procedure allows Sulzer Innotec to provide its customers with high-quality consultation on their engineering and on the optimization of their equipment.

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A Particle trajectory—left, small particles follow the main flow; right, large particles accumulate at the bottom of a channel.

