SIMULATION OF OFFGAS SCRUBBING BY A COMBINED EULERIAN-LAGRANGIAN MODEL

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ABSTRACT

In an industrial scrubber water droplets are introduced into the dust laden offgas in order to capture the fine dust particles. If the offgas stream is additionally guided through a contraction (e.g. a Venturi), the dust capturing efficiency is further increased because of the larger relative velocities between dust and droplets and the reduced droplet sizes. From a physical point of view the scrubbing process comprises a whole set of phenomena starting from droplet break-up and coalescence to the behaviour of the wall film and the dust capturing mechanism itself. The aim of this study is to address these phenomena by dedicated sub-models and incorporate them into a comprehensive simulation model within the OpenFOAM framework. Thereby, representative droplets are traced in a Lagrangian frame of reference while the fine dust particles are treated as additional passive Eulerian phases being allowed to drift with respect to the gas phase. Dust phases’ diffusivity is computed from its diameter and the local turbulence characteristics. Droplet break-up is considered by the Taylor Analogy Breakup (TAB) model. Dust capturing is triggered by impaction, interception and diffusion mechanism. In a further step the influence of a wall film is considered by a model extension solving the shallow water equations at wall boundaries. It is shown that on principle, modelling droplet deposition to the film is feasible as well as modelling droplet entrainment from the film due to film detachment and wave cresting. For the case without wall film numerical results are in good agreement with measurements found in literature as well as with a one-dimensional calculation approach that has been previously developed by the authors.

NOMENCLATURE

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INTRODUCTION

Due to the increasingly restricting legislation for the emission of pollutants there is a necessity for improved cleaning devices. Among the equipment utilised for cleaning of gases prior to release into the atmosphere, a Venturi wet scrubber, is one of the most effective. It can remove particles suspended in gaseous streams, achieving very high efficiencies even for particles of the order of micrometers (Dullien, 1989).

In Fig. 1 a Venturi scrubber is sketched. On principle, it comprises a convergence, a throat, and a diffuser. Dust laden gas enters the Venturi scrubber and accelerates in the convergence section. Due to the fact that the dust particles are very small they follow the gas stream nearly ideally. In the throat, the scrubbing liquid is injected and accelerated through drag force acting on the liquid droplets. As a result of the relative velocity between the droplets and the dust particles collisions occur and therefore the dust is captured by the droplets. The main collision mechanism in a Venturi scrubber is inertial impactation. Other collision mechanisms, such as interception and Brownian diffusion, are insignificant in comparison with inertial impactation (Boll, 1973). In a subsequent cyclone separator the droplets, whose diameters are much larger than the dust particles', can be removed from the gas stream.

Figure 1: Principle sketch of a Venturi scrubber.

Venturi scrubbers can be classified as either a liquid injection type (Pease–Anthony type) or a wetted approach type according to how the liquid is supplied (Pulley, 1997).

In the Pease-Anthony scrubber the scrubbing liquid is injected through orifices which are located at the throat. The injected liquid jet breaks up due to aerodynamic forces acting between the droplets and the gas. In the wetted approach type scrubber the liquid is introduced as liquid film that flows along the wall. In that case droplets are entrained into the gas stream due to shear force acting between the gas and the liquid film.

The main drawback of a Venturi scrubber is its large power consumption for operation which is determined by the pressure drop. As Gonçalves (2001) pointed out, many computational models are available for the prediction of pressure drop in Venturi scrubbers. One of the early models was presented by Calvert (1970). It assumes that there is no heat transfer between gas-walls, gas-droplets and gas-dust. The latter two assumptions postulate that the gas and the droplets (or dust particles) are at the same temperature which presumes a strong thermal coupling between the gas and droplet (or dust particle). Thus, in the following modelling both droplets and dust particles are assumed inert and isotherm.

The conservation of mass of the gas phase can be written as:

\[
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g) = 0. \tag{1}
\]

From the conservation of momentum one can derive:

\[
\frac{\partial (\rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g \mathbf{u}_g) = -\nabla p + \nabla \cdot \mathbf{\tau} + \rho_g \mathbf{g} + \mathbf{S} \tag{2}
\]

with

\[
\mathbf{\tau} = \eta_G \nabla \mathbf{u}_g + \eta_d \nabla \mathbf{u}_g + \eta_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d.
\]

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denoting the gas-phase stress tensor that accounts for an additional eddy viscosity $\eta_{G,t}$, here modelled using a k-ε turbulence model. Above equations are discretized and solved using a PISO-method (Pressure Implicit with Splitting of Operators) as described by e.g. Jasak (1996).

**Lagrangian model for droplets**

Since it is impossible to calculate the trajectory of every single droplet within an acceptable time, a simplification is made. Instead of individual droplets computational ‘parcels’ are traced with each parcel representing a certain mass of droplets that share the same properties (size, velocity, etc.). One could imagine each parcel representing the centre of mass of a cloud of equal droplets.

For the calculation of a parcel’s trajectory a simplified BBO-equation (Basset, Boussinesq, Oseen) is solved:

$$m_0 \frac{du_p}{dt} = -\mathbf{G} \mathbf{u}_p + C_{d,d} \rho_p \frac{\rho_p}{\rho_g} (\mathbf{u}_g - \mathbf{u}_p) \left( \mathbf{u}_g - \mathbf{u}_p \right).$$

If the particle and droplet loading is low, which can be assumed in most regions of a Venturi scrubber, the volume occupied by the particles can be neglected. Therefore, the gas phase and the droplets are coupled solely by a source term in the gas momentum balance (2) and a drag term in the parcels force balance (3).

**Droplet deformation model**

As observed by Alonso (2001) droplet size distribution changes along a Venturi scrubber which has a large effect on pressure drop as well as dust capturing efficiency. The change of droplet size is mainly triggered by droplet break-up and coalescence. In the present work models for both effects are applied.

![Figure 2: Axisymmetric representation of an oscillating, distorted droplet.](image)

**Droplet oscillation and break-up**

Initial droplets are formed due to primary break-up of a jet or a film. As a result of the shear forces acting on these droplets, they deform and break-up into smaller droplets. A well known model for droplet break-up is the Taylor Analogy Breakup (TAB) model described by O’Rourke (1987). The model is based on Taylor’s analogy between an oscillating, distorting droplet and a spring-mass-damper system, where the forcing term is given by aerodynamic forces, the damping is due to liquid viscosity and the restoring spring force is supplied by the surface tension. In this model the droplet’s deformation can be determined at any given time by solving a linear differential equation. The deformation of a droplet is described by the deformation parameter $y = \frac{2\Delta r}{r}$ as sketched in Figure 2.

Here, $\Delta r$ denotes the deformation of the droplet’s equator from the equilibrium position and $r$ the droplet radius. Actually, break-up occurs if the deformation reaches a critical value. Size and velocity of the subsequent child droplets can be determined from an energy balance.

As it can be seen in the droplet’s equation of motion, $C_{d,d}$, the drag coefficient of a droplet is needed for the computation of a droplet’s trajectory. For high Weber numbers droplets significantly deform, thus the assumption of a spherical droplet is no longer applicable. Following Taylor (1963), the shape of a deformed liquid drop can be regarded as a plano-convex lenticular body which has the same volume as the original body. The drag coefficient of a deformed droplet can be modelled as a linear interpolation between a sphere and a disc, depending on the droplet’s deformation,

$$C_{d,d} = C_{d,\text{shp}} (1 + 2.632y).$$

Within this work, the implementation of the TAB model as it is described in the KIVA-II manual, Amsden (1985), is used.

**Droplet coalescence model**

Besides droplet break-up, collision dynamics is important in the evolution of sprays. Hereby, O’Rourke’s (1981) model of droplet coalescence and grazing collision is commonly used. O’Rourke derived an equation modelling the collision probability on the basis of the assumption that the droplets are uniformly distributed inside the spray. Within this work once more, the implementation of Amsden (1985) is used.

**Modelling the dust phase**

For the modelling of the dust particles the dust phase is divided into dust fractions each representing a certain diameter. The concentration of each fraction is chosen corresponding to given size distribution function of the dust phase. Within this work the dust phase is regarded to have a log-normal distribution.

Due to the fact that the dust’s mass fraction is negligibly small it can be treated as an additional passive phase having no influence on the gas or droplets. Furthermore, since the dust particles have a very low relaxation time the dust movement is strongly coupled with gas flow. Nevertheless, the dust particles are allowed to drift with respect to the gas phase due to gravitational and centrifugal forces.

These assumptions lead to the following passive scalar transport equation for the dust concentration $\phi$ :

$$\frac{\partial (\phi \rho_d)}{\partial t} + \nabla \cdot (\rho_d \mathbf{u}_p) = D_{\text{diff}} \nabla^2 \phi$$

For the calculation of the dust fraction’s velocity $\mathbf{u}_p$ it is necessary to know $\mathbf{u}_{\text{Drift}}$, the drift velocity between gas and dust particles. Following the idea of Manninen (1996) the drift velocity $\mathbf{u}_{\text{Drift}}$ can be calculated from the gas velocity and the particle relaxation time as followed.
The force balance for a single dust particle can be written as

\[ m_p \mathbf{u}_p = m_p g - \frac{\rho_p \mathbf{u}_{\text{drift}}}{2} A_p \frac{24}{\text{Re}_p}. \]

Using the particle relaxation time, \( \tau_{p,\text{relax}} = \frac{\rho_p d_p^2}{18 \mu_G} \), above equation can be written as

\[ \dot{\mathbf{u}}_p = g - \frac{\mathbf{u}_{\text{drift}}}{\tau_{p,\text{relax}}}. \]  

Assuming local equilibrium one can assume that:

\[ \mathbf{u}_p = \left( \nabla \cdot \mathbf{u}_G \right) \mathbf{u}_G. \]  

Thus, using equations (7) and (8) the drift velocity can be calculated from the gas velocity and the particle properties.

The dispersion of particles strongly depends on the turbulence structure. According to Crowe (1985), the reciprocal Schmidt number denoting the ratio of diffusivity and effective viscosity is a function of the time ratio \( \tau_{p,\text{relax}} / \tau_{G,\text{turb}} \):

\[ \frac{D_\text{diff}}{\eta_i} = F \left( \frac{\tau_{p,\text{relax}}}{\tau_{G,\text{turb}}} \right). \]

Hereby, in RANS simulations using the k-ε turbulence model the characteristic time of large scale turbulent structures can be approximated as

\[ \tau_{G,\text{turb}} = 0.15 \frac{k}{\varepsilon}. \]

Thus, using above correlation the drift phases diffusivity can be calculated from turbulence parameters and the dust particles’ relaxation time.

**Modelling the capture of dust particles**

As Hähner (1994) pointed out, there are at least three mechanisms that might lead to deposition of dust particles (Figure 3) diffusion, impaction and interception.

**Impaction**

In literature many correlations for inertial drop collection efficiency are available (e.g. Pak, 2006; Pulley, 1997; Kim 2001). As a dimensionless number characterizing inertial collection a modified Stokes number is used,

\[ \psi = \frac{\rho_p d_p^2 |\mathbf{u}_G - \mathbf{u}_p|}{9 \eta_i d_D}. \]

An empirical correlation for the target efficiency for potential flow around a spherical droplet \( (\text{Re}_D \to \infty) \) is given by Langmuir, Pulley (1997)

\[ \eta_{\text{imp}} = \left( \frac{\psi}{\psi + a} \right)^b \]

with \( a = 0.5 \) and \( b = 2 \).

**Diffusion and Interception**

Within this work, models for diffusion and interception proposed by Jung (1998) are applied.

The total capturing efficiency is assumed to be the sum of the efficiencies due to impaction, diffusion and interception,

\[ \eta_{\text{tot}} = \eta_{\text{imp}} + \eta_{\text{diff}} + \eta_{\text{int}}. \]

Thereby, the number of particles captured by one droplet can be expressed as

\[ N_C = \eta_{\text{tot}} \frac{d_p^2 \pi}{4} |\mathbf{u}_p - \mathbf{u}_G| \Delta t \frac{N_p}{dV \Delta t}. \]

**Liquid Film Flow**

As Viswanathan (1998) pointed out, accounting for the liquid film flowing along the walls is necessary to accurately describe the physical phenomena occurring in a Venturi scrubber. The film influences the frictional pressure drop as well as droplet velocity and size distribution. Following Chengxin (1996) one can model liquid wall film using integral boundary layer type equations. With the help of boundary layer assumption and integral method, the three-dimensional Navier-Stokes equations can be reduced to two-dimensional equations defined on the wall boundary.

\[ \frac{\partial h}{\partial t} + \nabla \cdot (h \mathbf{u}_f) = \frac{S}{\rho_f} \]

\[ \frac{\partial \left( h \mathbf{u}_f \right)}{\partial t} + \nabla \cdot \left( h \mathbf{u}_f \mathbf{u}_f + C \right) = \frac{1}{\rho_f} \left( \tau_f - \tau_w \right) + h g - \frac{h}{\rho_f} \nabla \cdot p_f + \frac{S}{\rho_f}. \]

In above equations \( \mathbf{u}_f \) denotes the depth averaged film velocity. For the calculation of the shear stress terms and the convection correction tensor \( C \) a prescribed velocity profile is used. The film pressure \( p_f \), which is assumed to be constant over the film height depends on the gas pressure \( p_G \), the capillary pressure \( p_c = -\sigma \nabla \cdot \mathbf{n} \) and the droplet impact pressure \( p_{D,\text{impact}} \) with
\[ p_F = p_G + p_\sigma + p_{D,\text{impact}}. \]  

The film is coupled with the gas phase by the gas pressure and the shear force acting on the film surface \( \tau_f \). It must be remarked that this coupling acts only from the gas to the film but not the other way. If a droplet impinges on the film, its mass and its momentum are transferred to the film. The normal component of the momentum acts as a pressure term \( p_{D,\text{impact}} \) in the pressure equation, whereas the tangential term is added to the momentum equation. A limitation of the present model is the neglect of splashing caused by impinging droplets, this will be addressed in future work.

**Film Separation Model**

As it is described above the coupling between spray and film is accounted for by impingement mass, momentum and pressure. These terms model the influence of the spray on the film. In order to account for the influence of the film on the spray two models are implemented:

- A separation model, which covers the formation of droplets, when a liquid film flows over a sharp edge and separates.
- An entrainment model, covering the droplet entrainment due to gas shear forces acting on the film surface.

When a film flows around a corner it can either stay attached or separate and form droplets as sketched in Fig. 4. Due to inertia the film tends to keep its initial direction, thus at a corner a low pressure region establishes at the wall-side of the film. The pressure difference between the wall-side and the gas-side causes the film to stay attached on the wall. If the liquid inertia is so large that the wall-side pressure drops to zero, the film is believed to separate. Thus, O'Rourke (1996) postulated a separation criterion

\[ c_{\text{Sep}} \left( \frac{\rho_f}{\rho_L} \frac{\bar{u}}{v} \right)^{\frac{1}{2}} \sin(\theta) > p_G. \]  

**RESULTS AND DISCUSSION**

Using the models described in the preceding chapter a numerical analysis of a Pease-Anthony Venturi scrubber is carried out and the results are compared to measurements by Haller (1987). The geometry of the scrubber, depicted in Fig. 5, is discretized with ~100000 cells. A transient solver using the PISO algorithm is applied for the simulation. Time derivatives are discretized using an Eulerian scheme while Gaussian schemes are used for discretization of gradient and divergence terms.

The gas velocity in the throat is set to 70 m/s respectively 50 m/s and liquid/gas mass ratios ranging from 0.5 to 2.5 are considered for the calculation of the pressure drop and the grade efficiency. For the gas and liquid properties, those of air and water at 20°C and 1bar are used.

The liquid is injected through 12 orifices that are uniformly distributed along the circumference. The liquid inlet velocity is calculated from the flow rate and the orifice diameter of 2.5 mm. The initial droplet diameter follows a Rosin-Rammler distribution.

The dust is represented by 6 diameter fractions ranging from 0.1µm to 1µm. The fractions mass flow rates are obtained using a log-normal distribution and the total mass flow rate is set to 5e-7 kg/s.

In a first step the presence of a wall film is neglected and droplets colliding with the wall are reflected. Droplet break-up is modelled using the TAB model described in the preceding section. For cases with a higher loading than 2.0 the coalescence model by O'Rourke is applied.

**Film Entrainment Model**

As it was pointed out by Lopez de Bertodano (2001) the modelling of the entrainment rate of droplets from the liquid film is the greatest uncertainty in the film mass balance. Here the model of Taylor for the growth of ripples is applied to calculate an entrainment rate. As it was shown by Lopez de Bertodano the entrainment rate can be approximated by the following formula:

\[ \frac{\dot{D}_h}{\eta_L} \propto \frac{\rho_L \nu^2 D_h}{\sigma} \frac{\rho_L}{\eta_L} \nu_L \sqrt{\frac{\rho_L}{\rho_G}}. \]  

In contrast to other correlations proposed by Lopez de Bertodano, above formula does not need the ripple height to calculate the entrainment rate. Thus the ripples do not have to be spatially resolved in the simulation.
Pressure Drop

In Fig. 10 and 11 the calculated pressure drop is compared to that measured by Haller (1987) for throat velocities of 50 m/s and 70 m/s, and liquid to gas mass ratios ranging from 1 to 2.5. The overall pressure drop, as well as the pressure along the scrubber axis, are in good agreement to the measured data.

Capturing Efficiency

The capturing efficiency of different dust fractions is shown in Fig. 12. The calculation predicts a capturing efficiency of more than 99% for dust particles larger than one micron which is in good accordance with the data of Haller (1987). For smaller dust particles the capturing efficiency reduces dramatically. This is qualitatively the same behaviour as observed in the experiments. Nevertheless, the accuracy of the capturing prediction for high gas velocities is not yet satisfying.

Feasibility of a film model

In a second simulation step the feasibility of the film model should be shown by a simple test case that is inspired by the flow situation in a Venturi scrubber, depicted in Fig. 13. At position a) liquid droplets collide with the Venturi-wall and a liquid film is formed which flows, due to gravity and shear forces, down the walls. When the film reaches a sharp edge at position b) and the separation criterion (Eqn. 18) is fulfilled, the film separates and droplets are formed. These droplets are carried away by the gas stream. At position c) some droplets again collide with the wall and a film establishes again.

In Fig. 14 droplet entrainment from the film is shown. As in Fig. 13 a liquid film is formed by impacting droplets at position a). The separation at the sharp edge at position b) is neglected here and therefore the film flows further down the wall. If locally at position c) the entrainment criterion (Eqn. 20) is met, liquid droplets are formed and re-entrained to the gas stream.

A remaining weakness of this model is the need of an initial droplet size distribution. Although breakup and coalescence models are both applied, the pressure drop and the capturing efficiency strongly depend on that initial distribution. The amount of large droplets mainly causes the overall pressure drop, whereas the smaller droplets determine the capturing efficiency of small particles. Therefore, future work should concentrate on an improved prediction of droplet size distribution.
If a validation of the wall film – droplet interaction models succeeds it should be possible to simulate also wetted-type scrubbers where the liquid is injected as a film and droplets are subsequently formed by film breakup mechanisms.

CONCLUSION

A comprehensive model for the calculation of pressure drop and capturing efficiency of wet scrubbers has been developed and tested against experimental data. It models the gas phase as a continuous phase while the droplets are modelled in a Lagrangian frame of reference. The dust particles are treated as an additional passive Eulerian phase. Correlations for the capturing due to impaction, diffusion and interception are applied. Droplet size distributions are determined using a breakup- and a coalescence model.

Based on these models several operating conditions of a Venturi scrubber have been investigated. While the simulated pressure drops are in good quantitative agreement with experimental data the results for the capturing efficiency show reasonable tendencies. However, an accurate quantitative prediction of separation efficiency is not possible at the present stage.

Future work should concentrate on an improved prediction of droplet size distribution in order to enhance dust capturing calculation.

In a second part of the paper the feasibility of a liquid film model as well as its interaction with droplets and the gas phase has been shown. With this liquid film model it should be possible to investigate even scrubbers that are based on liquid film injection.

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