A simulation tool to predict spontaneous aerosol formation in gas-liquid contact devices

P. Hamberger, K. Schaber, D. Piccioni Koch,

Karlsruhe Institute of Technology, Karlsruhe, Germany

In gas-liquid contact devices like packed columns simultaneous heat and mass transfer take place and influence each other. Depending on the process conditions this can lead to a supersaturated state of the gas phase inside the device. When additionally solid particles are present, all perquisites for heterogeneous nucleation are fulfilled and aerosol formation can be observed (*Schaber, 1995*). The aerosol droplets are dispersed in the gas phase and are dragged along the device with the gas. When entering an undersaturated area inside or outside the device, the droplets evaporate again and thus have the potential to significantly influence the outcome of a process.

The simulation tool AerCoDe

The Institute for Thermodynamics and Refrigeration and the Steinbuch Centre for Computing at KIT are working on a simulation tool to model the heat and mass transfer in gas-liquid contact devices including the formation and growth of aerosol droplets. The model is based on the balance equations for mass and energy in the gas and liquid phase as well as in the aerosol droplets (Ehrig *et. al.*, 2002). The separate phases are connected by heat and mass transfer equations varying with the considered type of contact device. This yields mathematically a system of partial differential equations combined with additional algebraic equations. The time depended equations are initialized in a quasi-equilibrium state and integrated until the stationary state of the device is reached. The simulation tool is capable of predicting the saturation along the gas-liquid phase interface area and gives information on the droplet size, composition and temperature of the aerosol, that is formed inside the contact device. In undersaturated conditions, the code can simulate the evaporation of droplets. Recent upgrades also allow use multi-substance mixtures and polydisperse nucleation with different solid particles.

Application example: Double-stage acid recovery

In order to separate hydrochloric acid from flue gas after waste incineration, a double-stage scrubbing processes as shown in Figure 1 could be used. In the first stage the main part of the acid forming substance is absorbed in a highly concentrated circulating acid. At an acid mass fraction of 15% and a temperature of 50 °C, the vapor pressure of the acidic component cannot be neglected. Even when assuming equilibrium at the outlet, the gas is leaving the first stage loaded with 800 mg/m³ of the pollutant. The second stage is operated with pure water or a low concentrated acid, supersaturation and consequently aerosol formation occurs. When neglecting the aerosol in the column design, hardly any chlorine is predicted to be present in the exhaust gas. But when taking into account, that acidic droplets are dragged along with the gas, the AerCoDe simulations show pollutant loads of 5 mg/m³ up to 15 mg/m³. Furthermore with the simulation tool other scrubbing liquids like caustic solutions can be examined. This helps to find an operation state, where supersaturation and thus aerosol formation is completely avoided.

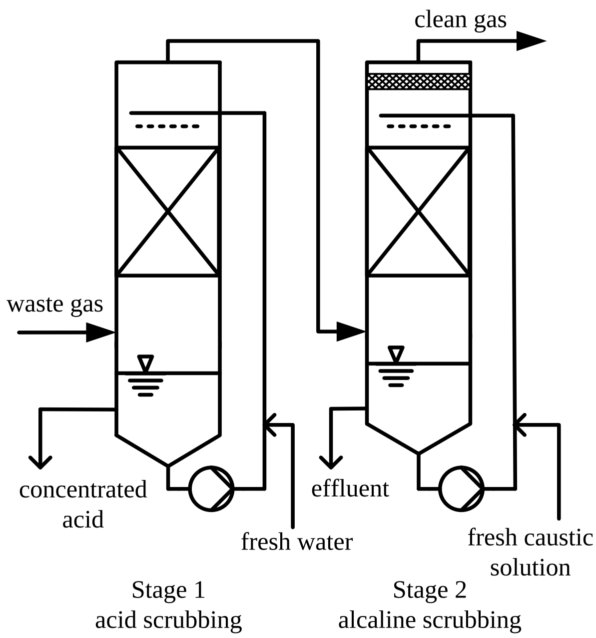

Figure 1. Scheme for a gas cleaning process with acid recovery using two serial wet scrubbers.

Literature

Schaber, K. (1995) *Chem. Eng. Sci.* **50**, 1347-1360.

Ehrig, R., Ofenloch, O., Schaber, K., Deuflhard, P. (2002) *Chem. Eng. Sci.* **57**, 1151-1163.