Mathematical Modeling of Atomizing Scrubbers

A mathematical model for predicting particle collection efficiency in an atomizing scrubber has been developed. The model solves the diffusion equations for both droplets and particles by using particle in cell technique. The effect of scrubber size and water distribution from various points of injection have been studied on collection efficiency. The results of the mathematical prediction agrees very well with the data reported in the literature for a wide variety of operating conditions and configurations.

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SCOPE

The simplicity of atomizing scrubbers has led to their emergence as one of the most widely used pieces of equipment in removing small particles from a gas stream. Atomizing scrubbers have been studied by many investigators and over the last 20 years a number of methods have been developed for predicting the collection efficiency as a function of operating variables (Johnston et al., 1954; Calvert, 1968; Boll, 1973). All make the assumption that the concentration of water droplets across the cross section of scrubber (perpendicular to the flow) is uniform. However, actual photographs and measurement of water droplet concentration across the throat taken by Taheri and Haines (1969) indicate that the droplet concentration across the throat is far from being uniform. Therefore, in any realistic model, the effect of droplet concentration distribution on particle collection efficiency should be taken into account.

The purpose of the present study was to develop and test a mathematical model for predicting the collection efficiency as a function of operating conditions. The main difference between this model and the previous one is that this model first predicts the concentration distribution of water droplets from a specified source of water droplets at the entrance instead of assuming a uniform water droplet concentration over the cross section. In other words, this paper develops a model which is capable of taking into account the geometry and size of the scrubber, method of water injection, and other operating variables.

The study of pressure drop across the scrubber is excluded from this study. Theoretically, pressure drop is independent of concentration distribution of water droplets and the model proposed by Boll (1973) can be used with confidence for the design purpose.

CONCLUSIONS AND SIGNIFICANCE

A mathematical model was developed for predicting particle collection efficiency in an atomizing scrubber. The model emphasizes the importance of water droplet concentration distribution on particle collection efficiency. The model was applied to predict collection efficiency and droplet concentration distribution as reported by various investigators. Excellent agreement between experimental data and theory lend strong support to the approach of using droplet concentration distribution as predicted by the diffusion equation for an estimation of collection efficiency.

MATHEMATICAL FORMULATION OF THE MODEL

Description

In an atomizing scrubber, liquid is atomized by high velocity air at the entrance of the scrubbing zone. The present model is based on the role of turbulence in mixing water droplets with the gas stream. For particulate matter, the material transport between the gas and liquid phase takes place in two steps. In the first step the eddy activity in the main stream serves as a transfer mechanism for moving the particles and water droplets close to each other. In the second step, the short-range mechanisms, such as the inertial impaction, transfer the particles to the water droplets. The short-range mechanisms and its effect on particle collection have been studied in great detail by a large number of investigators. However, very little attention has been given to the effect of the eddy activity on the mixing of water droplets with the gas stream. The present model is formulated based on the mixing process of the water droplets with the gas stream as a necessary step before short-range mechanism can become effective.

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Transport Equations

The coordinate system and the configuration of the scrubber are shown in Figure 1. The origin is placed at the center of the entrance cross section of the duct. The coordinate axis x is in the direction of the flow or along the axis of the duct, whereas y and z are perpendicular to the walls of the duct. The gas carries particulates into the duct and the particulates will be collected by the water droplets which are injected into the duct through a set of injectors. The equations for predicting the transport and diffusion of the particles and water droplets are as follows:

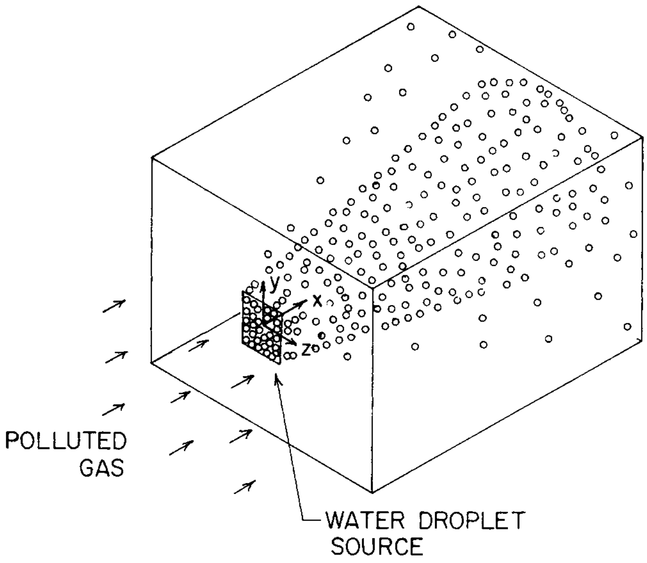

Fig. 1. Configuration and coordinate system of the scrubber atomizer.

$$\frac{\partial C_p}{\partial t} = -U_g \frac{\partial C_p}{\partial x} + E_p\left[\frac{\partial^2 C_p}{\partial y^2} + \frac{\partial^2 C_p}{\partial z^2}\right] - \frac{\pi \eta_t}{4} D_d^2 (U_g - U_d)\, C_p C_d \quad (1)$$

$$\frac{\partial C_d}{\partial t} = -U_d \frac{\partial C_d}{\partial x} + E_d\left[\frac{\partial^2 C_d}{\partial y^2} + \frac{\partial^2 C_d}{\partial z^2}\right] + Q_d \quad (2)$$

where C is the concentration, E is the eddy diffusivity, U is the velocity, Q is the source strength, η_t is the collection efficiency for a single drop, and D is the diameter. The indices d, p, and g are used to represent water droplets, particulates, and gas, respectively, throughout the paper. Equation (2) is valid for a concurrent atomizer, where the liquid is injected in the direction of gas flow. For this case the liquid momentum in the y or z directions was omitted and a distributed area source was chosen as a starting step. For a cross-current atomizer where the liquid is injected in the y or z directions, one can either include the appropriate terms in Equation (2) or treat the source of liquid as a line source in the y or z directions. Although this procedure may not be valid for all cases met in actual practice, it was found that the predicted results compared well with the limited available experimental data. In computing the above equations one must obtain expressions for the water droplets velocity, eddy diffusivity, target collection efficiency, and droplet diameter. These variables are discussed in the following sections.

WATER DROPLET VELOCITY

The water droplet velocity U_d is adjusted to the ambient air stream velocity according to the following equation:

$$\frac{dU_d}{dt} = \frac{3\rho_g (U_g - U_d)^2 C_D}{4\rho_d D_d} \quad (3)$$

where C_D is the drag coefficient, which, for an accelerating drop, a linear approximation of data reported by Ingebo (1970) is given by Calvert et al. (1972) as follows:

$$C_D = \frac{55}{Re} \quad (4)$$

where Re is Reynold's number. By substituting Equation (4) into Equation (3) one obtains an equation for the motion of water droplets:

$$\frac{dU_d}{dt} = \frac{41\, \mu_g (U_g - U_d)}{\rho_d D_d^2} \quad (5)$$

where U_g *is* the gas viscosity.

EDDY DIFFUSIVITY

The eddy diffusivity E depends on the flow situation and is a function of the degree of turbulence and mixing. Consequently it varies in different systems. Because of the lack of theoretical methods for predicting eddy diffusivity, it must be directly measured or estimated from empirical correlations. The compilation and correlation of eddy diffusivities has been underway for many years, but there are still many gaps to be filled. From literature (Himmelblau and Bischoff, 1968) it is generally accepted that for various systems at high Reynold's number, the ratio of $E/U\, D_t$ is a constant (D_t is the tube diameter and U is the fluid velocity). Therefore, by estimating this ratio for a particular size scrubber, one can predict the eddy diffusivity for other sizes. In the present development it was assumed that in an atomizing scrubber

$$\frac{E_g}{U_g D_t} = 0.1 \quad (6)$$

where E_g is the eddy diffusivity for the gas stream. The above equation and other empirical correlations given in the literature are usually valid for gases whose density is equal or close to that of the turbulent stream. Large particles and droplets, because of their inertia, cannot follow the random motion of eddies as easily as gases can. As a result, their eddy diffusivity is reduced. The effect of inertia on eddy diffusivity has been studied by Longwell and Malcolm (1953). These authors have assumed that the velocity fluctuations in the turbulent flow are sinusoidal and that Stoke's law applies to the drag on particles and drops. They obtained the following equation which was used in the present model:

$$\frac{E_d}{E_g} = \frac{b^2}{\omega^2 + b^2} \quad (7)$$

where E_d/E_g is the ratio of eddy diffusivity of the drop to that of the gas, $b = 18\mu/\rho_p D_p^2$ and ω is the frequency of the fluctuation of the turbulent air in radians per second.

COLLECTION EFFICIENCY

The mechanism of particle collection by atomizing scrubbers has been studied by many investigators and it is generally accepted that for particles above 0.5 μm the inertial impaction is the only important mechanism for removal of particles by water droplets. The collection of particles by single drop is calculated by the following equation:

$$\eta_t = \left(\frac{k}{k + 0.7}\right)^2 \quad (8)$$

This equation has also been used by other investigators including Calvert et al. (1972). In the above equation, η_t is target efficiency and k is the inertial impaction parameter and is given by Equation (9),

$$k = \frac{\rho_p D_p^2 (U_g - U_d)}{9\, \mu_g D_d} \quad (9)$$

For calculating the above parameter, the drop diameter D_d is an important variable. The correlation given by Nukiyama and Tanasawa (1938) is widely used to predict the drop size produced by atomizing scrubbers (see for example Calvert et al., 1972; Boll, 1973). The correlation for standard air and water is as follows:

$$D_d = \left[\left(\frac{5000}{U_g - U_d} \right) + 29 \left(\frac{1000\, Q_w}{Q_g} \right)^{1.5} \right] \quad (10^{-6}) \tag{10}$$

where Q_w/Q_g is the ratio of water to the gas flow rate.

NUMERICAL SOLUTION

Equations (1), (2), and (5) are the main equations for the present model. Equation (5) is integrated analytically and the droplets velocity U_d is computed. With all the other parameters known, the problem is then reduced to solving C_d and C_p from Equations (1) and (2). The numerical scheme applied is particle-in-cell developed by Sklarew (1972).

The initial distribution of the particulates is assumed to be uniform throughout the whole duct, and the initial concentration distribution of water droplets is assumed to be Gaussian plume as follows:

$$C_d = \frac{Q}{2\pi\sigma_y\sigma_z U_d} \exp\left\{ -0.5 \left[\left(\frac{y - y_s}{\sigma_y} \right)^2 + \left(\frac{z - z_s}{\sigma_z} \right)^2 \right] \right\} \tag{11}$$

where σ_y and σ_z are the standard deviation of horizontal droplet concentration in the plume. The coordinates x_s, y_s, z_s are the center of the water droplet source. The standard deviations in y and z directions are assumed to be equal and are expressed as follows:

$$\sigma_y = \sigma_z = [2E_d\,(x - x_s)/U_d]^{0.5} \tag{12}$$

In computing the concentration with Equation (11), the walls of the duct were treated as a perfect reflector, that is, an image source was added to the other side of each wall. The purpose for such an elaborate initialization is to make a better estimation of the distribution, thus reducing the time steps for the solution of the finite difference equation of diffusion by iterations. It should be noted that the final steady state solution should be independent upon the initialization if the number of iterations is large enough.

The boundary conditions are that the fluxes are zero at the walls and that the value of C_d and C_p are fixed at the entrance cross section. The boundary conditions at the downstream exit cross section are not needed because the scheme is essentially an upstream difference one.

Finally, the efficiency of the scrubber with the length L_x is computed from the ratio of the net amount of particulate material captured to the total amount of input. Assuming the same velocity at the inlet and outlet of the scrubber, one obtains the following expression for the overall efficiency:

$$\Psi = 1 - \frac{\iint C_p(L_x, y, z)\, dydz}{\iint C_p(0, y, z)\, dydz} \tag{13}$$

where the integration is computed for the entire cross section.

RESULTS

Useful data on atomizing scrubbers which can be used for testing a theoretical model are very scarce. Data given by a number of investigators were found to be of a limited value for testing the present model because the important items such as method of water injection, particle size, and scrubber size were generally lacking. Therefore, the model was tested with some limited experimental data which has been obtained under controlled conditions.

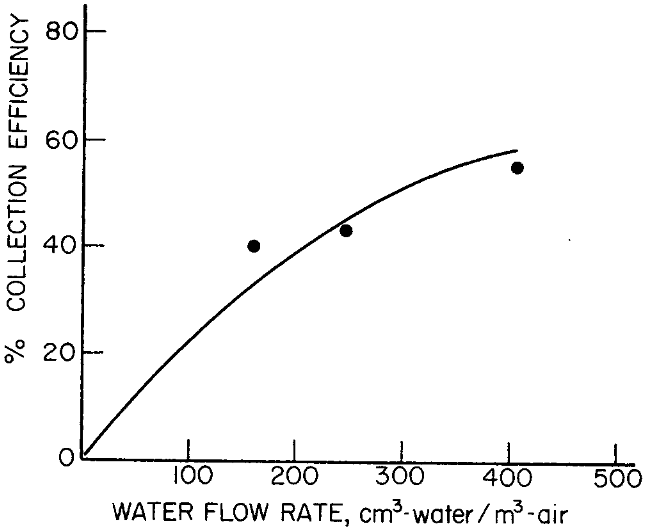

Fig. 2. Comparison of Calvert et al. particle collection data with the present model.

Certain input data to the model such as the dimension of the injector and velocity of the water injection were estimated from the available experimental knowledge. These values were assumed to remain constant for any given scrubber.

Particle Collection Efficiency vs. Water Flow Rate

Calvert et al. (1972) have reported experimental data on particle collection efficiency in a 10 cm × 30 cm rectangular cross section. The present model was tested by using the venturi dimensions and operating condition for experimental runs carried out with methylene blue aerosol. Only tests with methylene blue aerosol were considered because particles of this material do not change in size with humidity, and therefore the particle size reported at the scrubber inlet would represent the true particle size within the atomizing scrubber. Figure 2 compares the experimental collection efficiency for different water to gas ratios with the corresponding theoretical values predicted by Equations (1), (2), (5), and (13). The excellent agreement between the experimental and theoretical values of collection efficiency demonstrates the validity of the present model.

Particle Collection Efficiency vs. Particle Size

Brink and Contant (1958) have reported collection efficiency versus particle size in an industrial venturi scrubber. The scrubber used in their experiment had a 15 cm × 86 cm rectangular cross section with a straight section 30 cm long. The divergent section had an angle of 2.2° for 1.5 meter, following the venturi. The liquid was introduced into the gas stream through 45 spray jets across the 15-cm throat dimensions. Collection efficiency for phosphoric acid mist was obtained by measuring the particle size distribution and total loading at the inlet and outlet of the scrubber with a cascade impactor. For analysis of these data a line source of liquid was used as a starting step. Therefore, the initial momentum in the z direction was not considered. Numerically it was found much easier to handle a line source than to include the velocity terms in the z direction. The theoretical prediction and actual measurement is shown in Figure 3. Again the prediction by the present model agrees well with the actual measurement. In order to emphasize the effect of water droplet concentration distribution on collection efficiency, the results of a prediction assuming uniform droplet concentration distribution

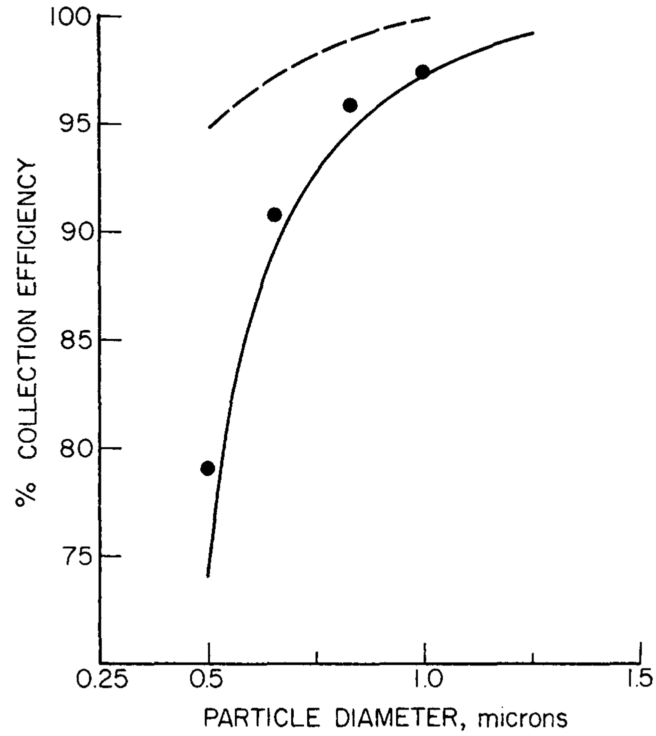

Fig. 3. Comparison of Brink and contant grade efficiency data with the present model: — present model, —— uniform droplet distribution model.

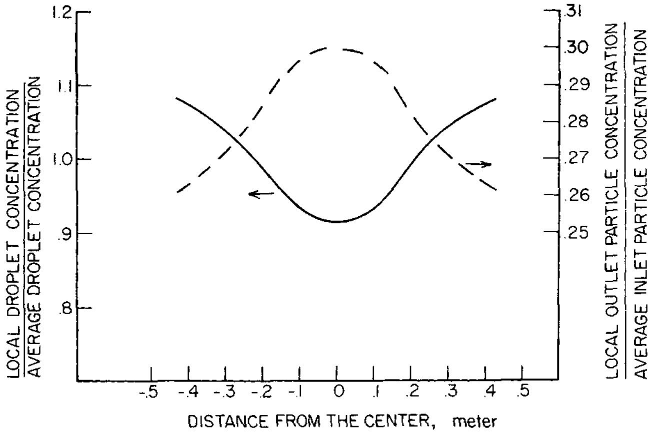

Fig. 4. Theoretical concentration distribution of drops and particles in Brink's venturi scrubber as a function of z at $y = 0$: — droplet profile, —— particulate profiles.

as given by Boll (1973) are shown on the same figure. It is clearly indicated that the model based on uniform water droplet distribution predicts higher collection efficiency than the experimental value. Calvert (1972) has introduced an empirical factor into the collection efficiency equation for a single drop to account for deviation from uniform concentration of water droplets.

The theoretical concentration distribution of the water droplets for the venturi scrubber of Brink under the same operational condition at a cross section approximately 20 cm below the spray nozzle is shown in Figure 4. This figure indicates that the concentration of water droplets at the nozzle's side is higher than the concentration in the middle of the venturi scrubber. Photographs of water droplet population distribution in an atomizing scrubber taken by Taheri and Haines (1969) and Boll (1973) indicate a similar pattern where the concentration along y axis (parallel to the nozzles) at the center of scrubber is considerably lower than the concentration at the nozzle's sides.

The variation in water droplet concentration distribution results in a change in particle concentration at the outlet of the scrubber. The profile of the penetration defined as the ratio of the outlet concentration to the inlet concentration is shown in the same figure. This profile indicates that at the middle of the scrubber, where a lower concentration of water droplets exists, the local penetration is higher than the corresponding nozzle's side. Because of the use of a large number of nozzles in y direction, no significant change in water droplet concentration or local penetration is obtained with respect to the y axis, and therefore the same profile is obtained for different values of y.

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NOTATION

- b = $18\mu/\rho_p D_p^2$, s^{-1}
- c_p = particulate concentration, g/m^3
- c_d = droplet concentration, number/m^3
- C_D = drag coefficient for drops, dimensionless
- D = diameter, m
- E = eddy diffusivity, m^2/s
- K = inertial impaction parameter = $\rho_p D_p^2 (U_g - U_D) / 9\mu_g D_d$, dimensionless
- L_x = scrubber length in the flow direction, m
- Re = Reynolds number (dimensionless)
- Q = source strength, number/m^3
- U = velocity, m/s
- x = rectangular coordinate, in the direction of the flow, m
- y = rectangular coordinate, perpendicular to the flow, m
- z = rectangular coordinate, perpendicular to the flow, m
- x_s = coordinate of the center of water droplet source in x direction, m
- y_s = coordinate of the center of water droplet source in y direction, m
- z_s = coordinate of the center of water droplet source in z direction, m

Greek Letters

- η_t = target efficiency for impacting particle on drops, dimensionless
- μ = viscosity, g/m s
- ρ = density, g/m^3
- Ψ = overall particle collection efficiency of the scrubber, dimensionless
- σ_y = standard deviation of horizontal droplet concentration distribution in plume in y direction, m
- σ_z = standard deviation of horizontal droplet concentration distribution in plume in z direction, m

Subscripts

- d = water droplets
- g = gas
- p = particulates
- w = water

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Prediction of Unsymmetric Convention Liquid-Phase Activity Coefficients of Hydrogen and Methane

A corresponding states method has been developed to predict the binary parameter in the unsymmetric-convention one-term Margules relation for binary activity coefficients of H_2 and CH_4 in solvents. In addition to the solvent density, only characteristic volumes used previously for partial molar volumes at infinite dilution and pure solvent compressibility are required. Comparisons with experiment for nonpolar solvents indicate that use of the method is usually significantly more accurate than assuming ideal solution (Henry's law).

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SCOPE

In the prediction of vapor-liquid equilibria in systems which contain supercritical components, such as hydrogen and methane at normal temperatures, there are special thermodynamic problems. Normal methods involve reference states requiring pure liquid phase properties which cannot be experimentally measured for these species and often are not conveniently obtained by extrapolation from data at temperatures below the critical. The usual approach is to use Henry's law where the reference state composition is infinite dilution of the supercritical component. While the assumption of ideal solution is satisfactory at very low concentrations of solute, it is less accurate as the concentration increases and activity coefficients in the unsymmetric convention must be used to account for deviations from ideality.

This work provides a method to predict such activity coefficients for hydrogen and methane in single solvents. It is a consistent extension of a corresponding states theory used previously for liquid compressibility and partial molar volumes of gases in solutions.

CONCLUSIONS AND SIGNIFICANCE

In general, the correlation [Equations (13) to (18)] requiring no additional binary information yields significantly more accurate results for bubble pressures and vapor mole fractions than does use of Henry's law in noncryogenic systems containing hydrogen and methane in nonpolar solvents. It is expected that the same should be true for polar solvents.

It has been well established that the unsymmetric convention is a convenient and accurate method for use in predicting vapor-liquid equilibria in systems containing substances which are significantly above their critical temperatures (Prausnitz, 1968, 1969). In general at moderate pressures, deviations from Henry's law are not great so that the data which are needed for liquid fugacities are Henry's constant at the temperature of the system and a convenient reference pressure, an approximate expression describing activity coefficients in the so-called "un-

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