ESTIMATION OF GAS CONCENTRATION FLUCTUATIONS USING A NUMERICAL MODEL AND COMPARISON WITH THOSE OF WIND TUNNEL EXPERIMENTS

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INTRODUCTION

In a hazard assessment of the accidental release of flammable or toxic materials into the atmosphere from a plant, it is important to consider not only the mean concentrations but also the fluctuation values of the pollutants. The instantaneous concentration is usually several times higher than time-averaged concentrations in atmospheric plumes and the prediction of only the mean concentration may significantly underestimate the potential hazard of the pollutants. A numerical model, which is based on the two-equation turbulence model for determining the turbulent kinetic energy and its dissipation rate, was applied to calculate the concentration fluctuations in a plume emitted from a point source near the ground. This model enables the solution of the transport equations not only for mean concentrations but also for the variances of concentration fluctuations. Numerical calculation results of mean concentration and the variances of concentration fluctuations were compared with those obtained using a high-frequency-response flame ionization detector in wind tunnel experiments, and three methods of estimating the dissipation time scale of concentration fluctuations were evaluated.

NUMERICAL MODEL

The turbulent transport of momentum is determined with the k-ε model based on the time-averaged partial differential equation. And the conservation equation for the concentration variances was used as the counterpart of the transport equation of the turbulent kinetic energy:

$$\frac{\partial \overline{c'^2}}{\partial t} + \frac{\partial \overline{u_i} \overline{c'^2}}{\partial x_i} = -2\overline{u_i' c'} \frac{\partial \overline{C}}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D \frac{\partial \overline{c'^2}}{\partial x_i} - \overline{u_i' c'^2} \right) - 2D \overline{\frac{\partial c'}{\partial x_i} \frac{\partial c'}{\partial x_i}} \tag{1}$$

where $\overline{u_i}$ is the mean velocity component in the x_i direction, u_i' is the fluctuating velocity component in the x_i direction, $\overline{C}$ is the mean concentration, c' is the fluctuating concentration and D is the molecular diffusivity.

Both the turbulent flux within the production term and the turbulent diffusion term of concentration fluctuations were modelled by the gradient transport hypothesis using the eddy diffusion coefficient. The dissipation term was modelled by the ratio of the concentration variance to dissipation time scale (Csanady, 1967):

$$-2D \overline{\frac{\partial c'}{\partial x_i} \frac{\partial c'}{\partial x_i}} = -\frac{\overline{c'^2}}{T_d} \tag{2}$$

where T_d is the dissipation time scale, T_d was estimated by using the calculated turbulent kinetic energy, its dissipation rate and plume length scale measured in wind tunnel experiments:

$$T_d = \frac{\sigma^2 \cdot \varepsilon}{2 \cdot C_\mu \cdot k^2} \tag{3}$$

$$\sigma = \alpha\sqrt{\sigma_z \times \sigma_y} \tag{4}$$

where k is turbulent kinetic energy, ε is the turbulent dissipation rate, C_μ is the empirical constant and taken from *Rodi*(1980) as 0.09, σ is the plume length scale (*Kouchi et al, 2000*), σ_z and σ_y are vertical and horizontal plume widths obtained from experimental results, respectively, and α is the model constant (=0.33). The calculation domains are 3.6m, 0.7m, and 1.0m for downwind (x), horizontal (y) and vertical (z) directions, respectively, and the computation is carried out with a 72 x 14 x 17 grid in the x, y, and z directions.

WIND TUNNEL EXPERIMENTS

The experiments were performed in the wind tunnel at Komae Research Laboratory of Central Research Institute of Electric Power Industry. The test section is 3m wide, 1.5m high and 20m long. A neutrally stratified boundary layer, which is 0.5m (=H) deep, was developed in the wind tunnel using roughness elements at the tunnel inlet. Measurements were carried out at a free stream wind speed of 1.0m/s (=U_e), and a tracer gas, a mixture of ethylene and air, was released from a ground-level point source, 5.0 x 10^{-3}m in diameter, and aligned with the flow, at the average flow velocity over its height.

Instantaneous concentrations were measured using a high-frequency-response flame ionization detector (FID) at several vertical cross sections downwind of the source. The sample gas emitted from a continuous point source was aspirated through a short, narrow metallic tube at a very high speed into the sampling chamber attached to the carriage system, which can be moved to arbitrary positions in the test section. An aspirated tracer gas was mixed with the fuel gas and burned in the chamber. The calibration of the detector was carried out using the test gas of known composition before each experiment and the detector was found to have linear calibration curves up to about 2,000 ppm. The detected signal was sent to a workstation that was outside the test section. The concentration data were obtained for 40 seconds at 2-millisecond intervals so that 20,000 data values were obtained at each measurement. To measure the mean and fluctuation velocity, a laser Doppler velocimeter (LDV) was also used. The schematic of the wind tunnel experiment is shown in Figure 1.

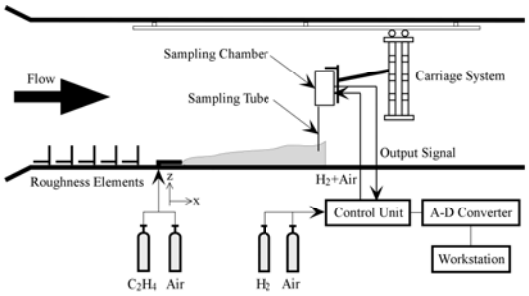

Figure 1. Schematic of the wind tunnel experiment.

RESULTS AND DISCUSSION

Vertical profiles of mean velocity and turbulent kinetic energy calculated at the position of the source, normalized by a free stream wind speed, are shown in Figure 2 with those obtained in wind tunnel experiments. Both mean velocity and turbulent kinetic energy profiles showed good agreement with measurements at the source position.

Vertical and horizontal plume widths are shown in Figure 3. Although calculated plume widths showed slightly larger values than those of wind tunnel experiments for vertical direction and showed slightly smaller values for horizontal direction, the calculations and measurements showed almost the same profiles.

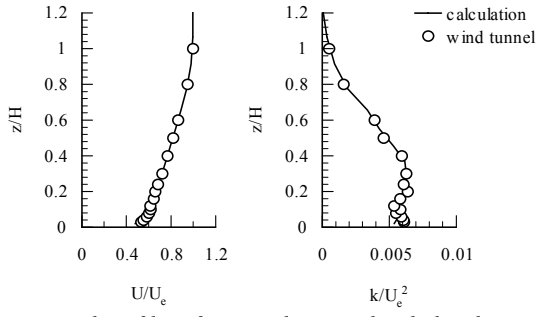

Figure 2. Vertical profiles of mean velocity and turbulent kinetic energy.

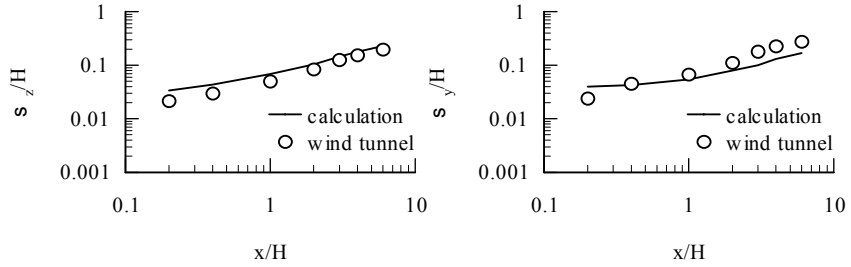

Figure 3. Vertical and horizontal plume widths.

Figure 4 shows vertical profiles of standard deviation of concentration fluctuations along with plume centerline at various downwind distances. The vertical profiles of standard deviation of concentration fluctuations showed forms similar to those of mean concentration, which are not shown in the figures, and the heights of the maximum for both mean concentration and concentration fluctuations were observed at the ground level. Although calculated standard deviations of concentration fluctuations were smaller than those obtained in wind tunnel experiments near the source, calculations showed good agreement with measurements taken far from the source. The dissipation term in the transport equation of concentration fluctuations is estimated using the plume length scale obtained in wind tunnel experiments as shown in Eqs. (2) and (3), so the concentration fluctuations are underestimated due to the very small plume length scale near the source. These disagreements did not occur far from the source because the plume disperses both vertically and horizontally and plume length scales used in the calculations were sufficiently large.

Horizontal profiles of concentration fluctuations are shown in Figure 5. Calculated fluctuations were also smaller than those obtained in the wind tunnel experiment near the source. This is due to the same reason as that given for the small vertical profiles. Modification is needed to estimate the dissipation time scale of concentration fluctuation accurately near the source where the plume does not grow sufficiently.

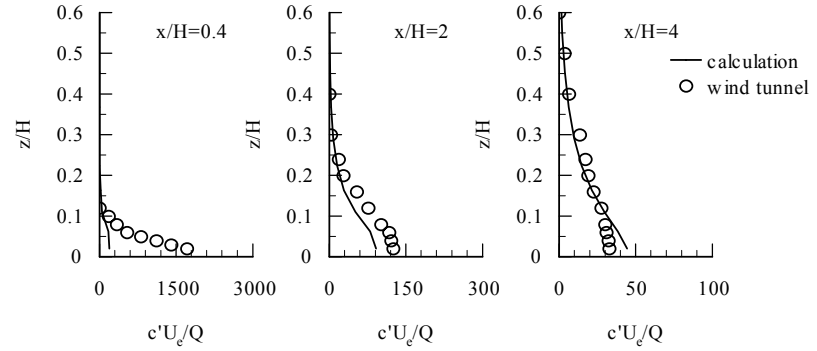

Figure 4. Vertical profiles of standard deviation of concentration fluctuations.

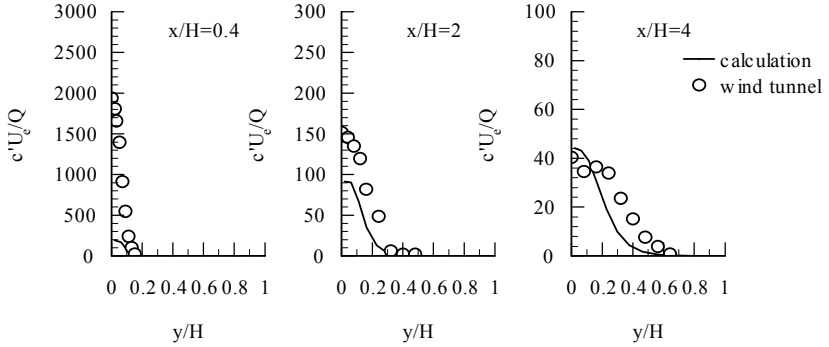

Figure 5. Horizontal profiles of standard deviation of concentration fluctuations.

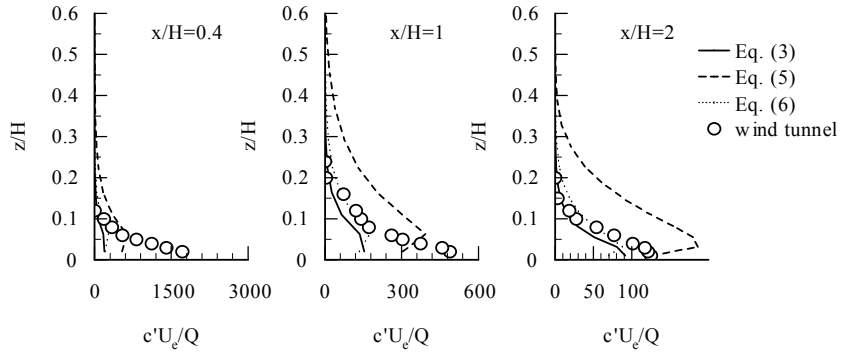

Figure 6. Concentration fluctuations calculated using Eqs. (3) and (6)

In addition to the method of estimating the dissipation time scale of concentration fluctuations using the plume length scale obtained in wind tunnel experiments (Eq. (3)), two other methods, i.e., Eqs. (5) (*Rodi,* 1980) and (6) (*Fackrell and Robins*, 1982), were used to estimate the dissipation time scale of concentration fluctuations:

$$T_d = \frac{R \cdot k}{\varepsilon} \tag{5}$$

$$T_d = \beta \frac{2\delta_z}{k^{1/2}} \tag{6}$$

where R is the time scale ratio and taken from *Ooka et al.* (1995) as 0.8, δ_z is the vertical plume half-width obtained from wind tunnel experiments, and β is the model constant (=0.25). Standard deviations of concentration fluctuations obtained using these methods are shown in Figure 6. It can be seen that all methods underestimate the concentration fluctuations that occur at ground level near the source. As the plume is carried downwind, Eq. (5) overestimates the measurements and the heights of the maximum concentration fluctuations were higher than those of wind tunnel experiments. This is because the dissipation term in the transport equation of concentration fluctuations is relative to the dissipation of turbulent kinetic energy that showed much larger values near the ground. Furthermore, concentration fluctuations were smaller at ground level than those at higher levels in the plume when the dissipation time scale was calculated using Eq. (5). The maximum heights of concentration fluctuations obtained using Eq. (6) were also observed a little higher than ground level near the source. In Eq. (6), the dissipation term in the transport equation of concentration fluctuations is relative to the square root of the turbulent kinetic energy that showed a peak value a little higher above the ground and heights of the maximum concentration fluctuations were also a little higher above the ground. Although it is difficult to compare absolute values of concentration fluctuations calculated using Eqs. (5) and (6) with those obtained from Eq. (3) directly because the model constant is included, the behavior of the concentration fluctuations near the ground obtained using Eq. (3) showed better agreement with measurements.

CONCLUSION

A numerical model based on the two-equation turbulence model was applied to calculate the concentration fluctuations in a plume emitted from a point source near the ground. The conservation equation for the concentration variances was used as the counterpart of the transport equation of the turbulent kinetic energy. Both the production term and turbulent diffusion term of concentration variances were modelled by the gradient transport hypothesis. The dissipation term was modelled using the calculated turbulent kinetic energy, its dissipation rate and plume length scale measured in wind tunnel experiments. Numerical calculation results of the mean concentration and the concentration fluctuations were compared with those obtained in wind tunnel experiments. Although there is a tendency that the model underestimates the concentration fluctuations near the source, the vertical profiles of concentration fluctuations showed better agreement with those of wind tunnel experiments when the dissipation time scale of concentration fluctuations was calculated using the plume length scale.

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