MODELLING AND SIMILARITY RELATIONS OF PHYSICAL AND CHEMICAL PROCESSES

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ABSTRACT

Proper modelling of chemical and physical processes of pollutants in the atmosphere and tests under controlled conditions may be made to complement field measurements in reducing the cost and time and the uncertainty due to changing meteorological conditions in field measurements. With knowledge gained from correlating model and field tests, proper modelling and model testing permit prediction and checking of performance of a given design of an emission source. The design parameters may include stack height, ejection speed, and its location with respect to buildings and topography. Proper modelling calls for design and testing based on accurate similarity relations. For gaseous or particulate components k in a gravitational field of acceleration g, hydrodynamic field of characteristic velocity U, electric field of characteristic potential V, and charge to mass ratio $(q/m)_k$ with reaction rate constant k_{jm} with components j's of number densities n_j's, surface interaction rate k_s with surfaces of area to volume ratio S_s, diffusivity D_k, characteristic dimension L, characteristic time t, primary similarity parameters are: (tU/L), $(\tau g/U)$, (D_k/UL), or (D_kt/L^2), (k_jn_jL/U), etc., (k_sS_sL/U) etc., and $(\tau_k(q/m)_k)V/LU)$. With programmed testing of a proper model, the diffusion phenomenon, for instance, over a year from an actual installation can be checked by one day of testing according to the parameter (D_kt/L^2) of model and prototype. Obviously, the above similarity relations cannot all be satisfied at once. A complete check on an installation would take several model tests. Specific cases and details discussed are: (a) actual stack plume rise based on Sutton's diffusivity as compared with wind tunnel test results which satisfy relations based on Tollmien's diffusivity; (b) diffusion and fall-out in relation to relaxation time; (c) correction for chemical reaction rates.

INTRODUCTION

The rate of transport, settling, diffusion and chemical and nuclear reactions of pollutants in the atmosphere have been subjects of intensive studies and observations[1]. The time and cost of field measurement and the difficulty in drawing definitive conclusions arising from changing meteorological conditions over durations of measurements are well known. Prediction of the consequence of introducing an emission source of a given design is largely a matter of conjecture. For a combination of stack height, ejection speed and location with respect to buildings and topography, prediction is hampered by the lack of an accurate mathematical model on the one hand, and lack of rigorous data on the other. It is therefore desirable to check a given installation with proper model testing in order to avoid costly corrections, technical or public relations wise, after it becomes operative. Even for an existing installation, proper modelling can reduce the cost and the duration of field measurements. Moreover, correlations of model and field results can sharpen future predictions from modelling.

By proper modelling is meant modelling based on accurate similarity relations according to fundamental principles. For instance, modelling of transient diffusion phenomena involves similarity based on (to be delineated later):

$$\frac{D_{\mathrm{M}}\, t_{\mathrm{M}}}{L_{\mathrm{M}}^2} = \frac{D_{\mathrm{P}}\, t_{\mathrm{P}}}{L_{\mathrm{P}}^2} \tag{1}$$

where D denotes diffusivity, t denotes time scale, L denotes characteristic length, subscripts M for model and P for prototype. It is seen that testing of a 1/1000 scale model in a wind tunnel such that $D_{\mathrm{M}} = D_{\mathrm{P}}/1000$ the time scale is reduced to 1/1000th of that of the prototype. Hence, what takes one day to observe in the field can be determined over 1·44 minutes. Programmed testing with varying meteorological conditions in a wind tunnel on a model mounted on a turntable can check conditions over a year in 8 hours and 45 minutes.

Complete testing of a given installation might call for several models over different scales of time, length, velocities and materials for various chemical and physical processes. Knowledge on model design has to be built up from basic testing under controlled conditions followed by evaluation and conversion to prototype conditions. In this paper, basic relations will be first delineated, followed by considerations of typical processes.

FUNDAMENTAL RELATIONS

General consideration of chemical and physical processes of pollutants in the atmosphere has to include transport and settling of aerosols and gaseous components, reacting or nonreacting, in gravitational, hydrodynamic, and electromagnetic fields. Extending the concept of multiphase systems[2], the density or concentration ρ_k of a species k in a principal fluid of density ρ is given by:

$$\frac{\mathrm{d}\rho_k}{\mathrm{d}t} - \rho_k \frac{\mathrm{d}\ln\rho}{\mathrm{d}t} = -\nabla\,.\,[\tau_k\, \rho_k\, F_k - D_k \nabla \rho_k] + \Gamma_k \tag{2}$$

where t is the time, τ_k is the relaxation time for momentum transfer between species k and the principal fluid, F_k is the force per unit mass acting on species k, D_k is its diffusivity, Γ_k is the rate of generation of k and

$$\Gamma_k = m_k\,[-k_1 n_k - \sum_j k_{2j} n_k n_j \ldots - \sum_s k_s n_k S_s] + m_k \sum_j k_{ij} n_j n_k \ldots \tag{3}$$

where m_k is its mass, n_k its number density; $\rho_k = n_k m_k$; k_1 is the rate constant for dissociation of k, k_{2j} that for second or higher order reaction with j etc. k_s for adsorption or reaction with surface s of surface area per unit volume S_s, k_{ij} is the rate for yielding species k.

Non-dimensionalizing of equations 1 and 2 gives the following primary dimensionless parameter for modelling, for characteristic dimension L, characteristic velocity U, characteristic time t_0, and acceleration of gravity g: $t_0\, U/L$, $\tau_k\, g/U$, D_k/UL or $D_k\, t_0/L^2$, $k_1\, n_j\, L/U$, etc.; $k_s\, S_s\, L/U$, etc.; and for charge to mass ratio $(q/m)_k$ in an electric field characteristic potential V_0, such as that due to the electric field in the atmosphere[3], we have

$$\tau_k V_0\, (q/m)_k/UL$$

Obviously, we cannot satisfy all similarities at once. The following sections illustrate the nature of similarity parameters of specific phenomena.

STACK PLUME RISE

A simple case of modelling an atmospheric process is that of the wind tunnel testing of the rise of a stack plume. It is seen that the controlled condition in a wind tunnel permits treating the plume as a turbulent jet. The boundary theory gave the centreline velocity w_0 as[4, 5]:

$$\frac{w_0}{w_1} = \frac{r_1\, w_1}{D} \left\{ \frac{3}{8}\, \frac{1}{(s/r_1)} + \frac{1}{8} \left[\frac{(T_1 - T_h)}{T_h}\, \frac{g r_1}{w_1^2} \right] \int_{(s_0/r_1)} \frac{d\,(s/r_1)}{(s/r_1)\,(w_0/w_1)} \right.$$
$$\left. - \frac{1}{8}\, g \left(\frac{\partial T}{\partial z}\right) \frac{T_1}{T_h^2}\, \frac{r_1^2}{w_1^2} \int_{(s_0/r_1)} \left(\frac{z - z_0}{r_1}\right) \frac{d\,(s/r_1)}{(s/r_1)\,(w_0/w_1)} \right\} \tag{4}$$

where D is the turbulent diffusivity, s is measured along the centerline with the mouth of the stack at $s = s_0 = (\sqrt{3}/2)\, \gamma\, r_1 = z_0$, r_1 is the radius of stack with exit velocity w_1, $\gamma = (\sqrt{3}/4)\, (r_1\, w_1/D)$, g is gravitational acceleration, T_1 and T_h are the temperatures of the stack gas and the ambient air at the stack exit, $(\partial T/\partial z)$ is the temperature gradient in the ambient air, z is the coordinate opposite to the direction of gravity, x is the coordinate normal to z in the plane of w_1 and cross (horizontal) wind of velocity u. Tollmien gave $D = r_1\, w_1/39$[6]. Equation 4 can be rewritten as:

$$\frac{w_0}{w_1} = \left(\frac{r_1\, w_1}{D}\right) \left\{ \frac{3}{8}\, \frac{1}{(s/r_1)} + \frac{1}{8}\, N_{Gr}' \int \frac{d\,(s/r_1)}{(s/r_1)\,(w_0/w_1)} \right.$$
$$\left. + \frac{1}{8}\, N_{Ri} \int \left(\frac{z - z_0}{r_1}\right) \left(\frac{d\,(s/r_1)}{(s/r_1)\,(w_0/w_1)}\right) \right\} \tag{5}$$

where N_{Gr}' is a modified Grashof number

$$N_{Gr}' = \left(\frac{T_1 - T_h}{T_h}\right) \frac{g r_1}{w_1^2} = \left[\frac{g\beta\,(T_1 - T_h)\, r_1^3}{D^2}\right] \left(\frac{D}{r_1\, w_1}\right)^2 \tag{6}$$

β is the coefficient of expansion of the gas, and N_{Ri} is the Richardson number

$$N_{Ri} = -\, g \left(\frac{\partial T}{\partial z}\right) \frac{T_1}{T_h^2}\, \frac{r_1^2}{w_1^2} = \frac{g}{\rho_1} \left(\frac{\partial \rho}{\partial z}\right)_0 \frac{r_1^2}{w_1^2} \tag{7}$$

where ρ_1 is the density of the exit gas, $(\partial\rho/\partial z)_0$ is the density gradient in the ambient air. The rise of the jet axis is given by:

$$dz = \sin\theta \, ds = [1 - (u/w_1)^2]^{\frac{1}{2}} \, ds \tag{8}$$

and the distance along the ground is given by:

$$dx = (u/w_0) \, ds \tag{9}$$

For small curvature of path, solution of equations 4 and 8 gives the plume rise along s and equation 9 gives the ground distance. For $w_1/u = 4$, and Tollmien's value for diffusivity, we get the following typical values of ultimate rise Δh from numerical integration until $dz/ds = 0$.

N_{Gr}'	N_{Ri}	$\Delta h/r_1$
3×10^{-3}	0	35·35
3×10^{-4}	0	32·54
3×10^{-4}	3×10^{-4}	32·94
3×10^{-4}	-3×10^{-4}	29·50
0	0	31·70

For the case N_{Gr}', $N_{Ri} = 0$, equations 4 and 8 can be solved analytically to give the maximum momentum rise. For comparison to previous results we choose the case $N_{Gr}' = 0$, $N_{Ri} = 0$. Based on constant turbulent diffusivity D, the maximum momentum rise Δh_v at $dz/dx = 0$ is:

$$\frac{16}{3}\,\frac{D}{r_1 w_1}\,\frac{\Delta h_v}{r_1} = \frac{u}{w_1}\left\{\frac{w_1}{u}\left(\frac{\pi}{2} - \sin^{-1}\frac{u}{w_1}\right) - \sqrt{\left[1 - (u/w_1)^2\right]}\right\} \tag{10}$$

at $x/r_1 \geqslant \frac{3}{8}\,\frac{r_1 w_1}{D}\left(\frac{u}{w_1}\right)\left(\frac{w_1^2}{u^2} - 1\right)$.

Equation 10 is presented in *Figure 1* and is identified as the boundary layer theory. This relation is compared to the Bosanquet relation[7] for stack volume emission rate of $Q_v = \pi r_1^2 w_1$ expressed in the form:

$$\frac{\Delta h_v}{r_1} = \frac{4{\cdot}77\,\sqrt{[\pi\,(w_1/u)]}}{1 + 0{\cdot}43\,(u/w_1)}$$

Also plotted in *Figure 1* are the experimental points of Bosanquet from field observation and wind tunnel results of New York University[8]. It is seen that the wind tunnel results conform to the boundary layer theory closely together with the condition of $\Delta h_v \to 0$ as $u \to w_1$. The Bosanquet relation gives a higher value of Δh_v for $w_1/u < 6$.

It is noted that the relation based on boundary layer theory is a consequence of Tollmien's D from wind tunnel tests. In atmospheric process, however, turbulent diffusion follows the Sutton relation[1], as

$$D_z = \tfrac{1}{4}\, C_z^2\, u\, x^{1-n}\,(2 - n) = \tfrac{1}{4}\,(C_z\, x^{-n/2})^2\, u\, x\,(2 - n) \tag{12}$$

where C_z is the Sutton's diffusion coefficient in (length)$^{n/2}$ and n is a turbulent index. In metric units, $0{\cdot}05 < C_z < 0{\cdot}58$, $0{\cdot}19 < n < 0{\cdot}58$. Since the

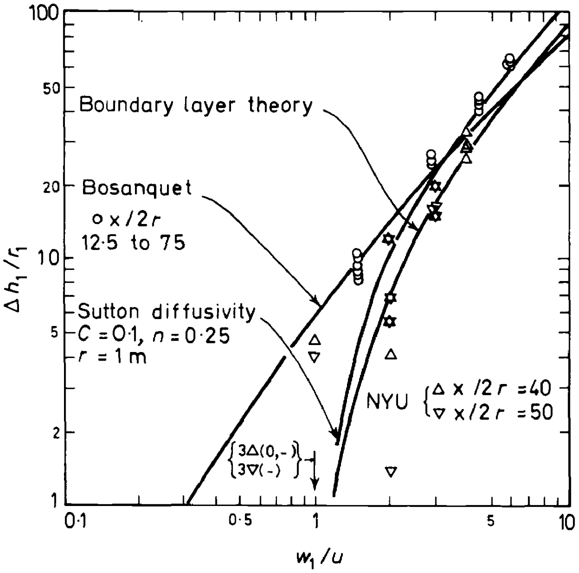

Figure 1. Comparison of wind tunnel and field tests of maximum momentum rise of stack plume and formulations.

atmospheric diffusivity increases with x, the relation between boundary layer and the atmospheric measurement in *Figure 1* is clearly consistent, with a ratio of Δh_v $_{\text{(measured)}}/\Delta h_v$ $_{\text{(B.L.)}}$ of 2·6 at w_1/u of 1·5 and 1·3 at w_1/u at 6. The inverse of this ratio of plume rise is the ratio of Sutton's to Tollmien's diffusivity. In this case, modelling clearly requires correction for turbulent diffusivity.

CONCENTRATION OF SPECIES

Sutton's diffusion equation is a solution of the diffusion equation for gaseous species of concentration ρ_k in the form[1]:

$$D_z \frac{\partial^2 \rho_k}{\partial z^2} + D_y \frac{\partial^2 \rho_k}{\partial y^2} = u \frac{\partial \rho_k}{\partial x} \tag{13}$$

with the condition $\partial \rho_k/\partial z = 0$ at $z = 0$ and $\pi r_1^2 \rho_{k1} w_{k1} = \int \int_{-\infty}^{\infty} \rho_k w_k \, dy \, dz$.

Here D_z, D_y are turbulent diffusivity in the z and y directions, the vertical and lateral directions, with motion in the x direction at velocity u. It takes the form, for u = constant:

$$\rho_k = \rho_{k1} \left(\frac{r_1}{x}\right) \frac{r_1 w_{k1}}{4 (D_y D_z)^{1/2}} \left[\exp\left(- \frac{y^2 u}{4 D_y x}\right) \right] \left\{ \exp \left[- \frac{(z - h)^2 u}{4 D_z x} \right] + \exp \left[- \frac{(z + h)^2 u}{4 D_z x} \right] \right\} \tag{14}$$

h being the height of the plume axis above ground, with turbulent diffusivities*:

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*Rigorous derivation of Sutton's equation requires $D_y = \frac{1}{4} C_y^2 u X^{1-n} (2 - n)$; $D_z = \frac{1}{4} C_z^2 u x^{1-n} (2 - n)$.

$$\left.\begin{aligned} D_y &= \tfrac{1}{4}\, C_y^2\, u\, x^{1-n} \\ D_z &= \tfrac{1}{4}\, C_z^2\, u\, x^{1-n} \end{aligned}\right\} \tag{15}$$

and h is the height of the axis of the plume above ground; ρ_{k1} is the concentration of species k at the source. Model testing requires that correction be made on $r_1\, w_1/(D_y/D_z)^{\frac{1}{2}}$ beside similarity of $L\, U/D$, L being the characteristic length of modelling.

For particulates (subscript p) gravity effect has to be incorporated. The diffusion equation including the gravity effect takes the form:

$$D_{pz}\, \frac{\partial^2\, \rho_p}{\partial z^2} + \tau_p g\, \frac{\partial\, \rho_p}{\partial z} + D_{py}\, \frac{\partial^2\, \rho_p}{\partial y^2} = u\, \frac{\partial \rho_p}{\partial x} \tag{16}$$

where τ_p is the relaxation time of momentum transfer to particles, g is the acceleration of gravity, $\tau_p g$ is the terminal velocity of fall. A solution of this equation was obtained by the following transformation of coordinates†:

$$\left.\begin{aligned} &\rho_p = e^{\,bz}\, e^{\,b^2\tau}\ F, \\ &\eta = y\ (D_{pz}/D_{py})^{1/2} \\ &\tau = (x/u)\ D_{pz},\ b = (\tau_p\ g/2D_{pz}) \end{aligned}\right\} \tag{17}$$

to give

$$\frac{\partial^2 F}{\partial \zeta^2} + \frac{\partial^2 F}{\partial \eta^2} = \frac{\partial F}{\partial \tau} \tag{18}$$

which has the solution

$$F = c \exp\left[\, - (\eta^2 + z^2)/4\tau\right] \tag{19}$$

c being the constant of integration which was determined in an analogous manner as in the Sutton equation. Equation 19 reduces to the Sutton equation for $\tau_p \to 0$. The mass flux at the ground due to fall-out is given by:

$$- J_p = - \tau_p\, g\, \rho_p\, (0) - D_{pz}\, \partial \rho_p/\partial z_0 \tag{20}$$

and g is replaced by $g + E_z\, (q/m)$ when particle charge is prominent; E_z being the electric field of the atmosphere.

The ground level flux can be expressed in terms of (for complete absorption at ground level):

$$J^* = \frac{J_p\, h^2}{\pi r_1^2\, \rho_1\, w_1} \left(\frac{4\pi\, u\, h}{D_{pz}}\right) \left(\frac{D_{py}}{D_{pz}}\right)^{\frac{1}{2}} \exp\left[\frac{y^2 u}{4 D_{py} x}\right]$$

$$\tfrac{1}{2} \left(\frac{\tau^* x^* + 1}{x^{*2}}\right) \exp\left[- \frac{(\tau^*\, x^* - 1)^2}{4\, x^*}\right] \tag{21}$$

where $\tau^* = \tau_p\, gh/D_{pz}$,

$x^* = D_{pz}\, x/h^2 u$

The relation given by equation 21 is shown in *Figure 2*. *Figure 2* shows that gravity effect is important only when the dashed line starts to bend from vertical. For $\tau^* < 1$ diffusion is unaffected by the gravity effect. For

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† Suggested by Professor B. T. Chan, University of Illinois.

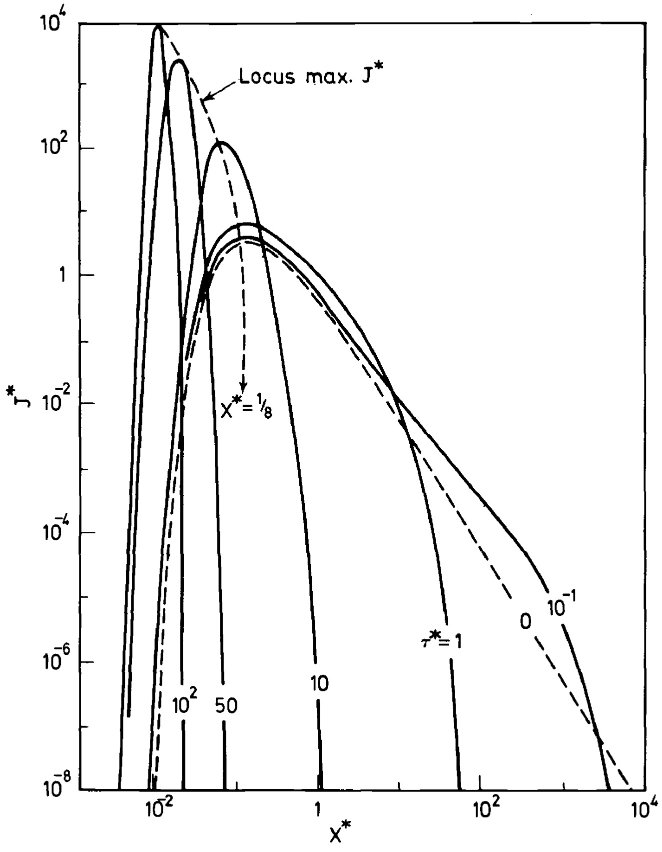

Figure 2. Fall-out correlation based on simultaneous effects of gravity and diffusion

$\tau^* < 1$, the trend of deposition function follows Bosanquet, *et al.*[1] However, *Figure 2* gives the local value of J. The importance of modelling based on similarity or correction of τ^* and x^* is seen. Physical magnitudes are $\tau_p \sim 4{\cdot}5 \times 10^{-10}$ sec and $D = 1{\cdot}21 \times 10^{-5}$ m^2/sec for SO_2 molecules in air at 300°K, $\tau_p \sim 3 \times 10^{-6}$ sec for 1μ water droplets and 3×10^{-2} for $10\,\mu$ flyash. Realistic simulation of fall-out rate can be made with due allowance for the diffusion effect.

When a distribution in particle size (radius a) exists such that the number distribution function at the source is known, an integration procedure can be applied[2].

Additional details of particulate systems in aspects of heat transfer and electric charge phenomena are treated in two recent reviews[9, 10].

CHEMICAL REACTION

Modelling of chemical processes in the atmosphere may include simulation with tracer species whose rates can be correlated according to the

Fundamental Relations. However, basic atmospheric processes of SO_2, N_2O, NO, NO_2, with O_2, O_3, and radiation and catalysis are not known in detail[1]. Selection of fast reactions for testing at reduced scale represents a challenging undertaking[11]. The use of natural composition for model testing raises difficulties from considering reported half-life of SO_2 of 43 days (corresponds to a rate constant of $2{\cdot}5 \times 10^{-7}$ m^3/kg mole sec and activation energy of 20 kcal)[1].

When simulation of physical process is satisfied, however, the effect of the chemical process can be computed. Take the example of a second order reaction in a diffusion process of component k of pollutant:

$$k\ \rho_k\, n_j + D_z \frac{\partial^2 \rho_k}{\partial z^2} + D_y \frac{\partial^2 \rho_k}{\partial y^2} = u \frac{\partial \rho_k}{\partial x} \tag{22}$$

for rate constant k and n_j moles/m^3 of j-th series. Computation is readily carried out with the perturbation:

$$\rho_k = \rho_k^{(0)} + (-k\, n_j)\, \rho_k^{(1)} + \dots \tag{23}$$

$\rho_k^{(0)}$ is the density of k-th series due to diffusion. It is seen that for small concentrations of ρ_k

$$\rho_k^{(1)} = \rho_k^{(0)}\, \mathrm{e}^{-kn_j x/u} \tag{24}$$

and correction from model testing result can be carried out.

CONCLUSION

The above considerations show that modelling and simulation of atmospheric processes are feasible. Care should be exercised, however, in interpreting wind tunnel test data. Complete simulation has to account for the detailed description of turbulence. Conversion to actual conditions can be made with model testing under various geographical and topological conditions. This is to be aided by the theory of imperfect modelling and correction of errors by machine computation[12], since equality of all similarity parameters of the model and the prototype can never be achieved in a single experiment. Extensions to general physical and chemical processes is desirable.

With the above examples, the basic considerations which have to be made in modelling and simulation are demonstrated. It is logical to visualize through the testing of a site with pollutant emission using several scale models with various time programmings for a complete study of the influence of an emission source on its surroundings.

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