UIT Report Vol. 13, No. 2, pp. 309~317, 1962　　연구논문집 제13권 제 2 호 pp. 309~317, 1982

Dispersion of Passive Contaminants in a Turbulent Boundary Layer

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(Received June 30, 1982)

〈Abstract〉

A method to predict the dispersion of passive contaminants in a turbulent boundary layer is developed based on second-order closure approach. The dissipation of the mean scalar flux due to pressure scrambling is assumed to be inversely proportional to the plume length scale when the plume scale is small. The result appears to be in general agreement with the experiment.

경계층 내에서의 난류 확산에 관한 연구

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〈要　約〉

경계층 내에서의 난류 확산을 해석하기 위한 새로운 second-order closure 방법을 개발 하였으며, 난류 경계층 내에 있는 점원으로부터의 확산에 관한 문제에 적용한 결과는 실험결과와 잘 일치하고 있다.

I. Introduction

Predicting the dispersion of passive contaminants in a turbulent boundary layer has a great importance with wide applications and has been worked out by several authors.

The boundary layer approximation of the transport equation for the mean concentration C is, neglecting the molecular diffusion,

$$U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}+W\frac{\partial C}{\partial z}=-\frac{\partial\overline{vc}}{\partial y}-\frac{\partial\overline{wc}}{\partial z}\quad(1)$$

Here x, y, and z are the Cartesian coordinates in the mean flow, vertical, and lateral direction respectively and U, V, and W are mean velocities in the x-, y-, and z-direction respectively, while $\overline{vc}$ and $\overline{wc}$ denote the mean fluxes of contaminants in the y- and z-direction due to the turbulent fluctuation.

One of the simplest and the most widely used approach is to relate the mean fluxes to the gradients of the mean concentration assuming the eddy diffusivies, i.e.,

$$\overline{vc}=-K_y\frac{\partial C}{\partial y},\quad \overline{wc}=-K_z\frac{\partial C}{\partial z}\qquad(2\text{a, b})$$

where K_y and K_z represent the eddy diffusivities in the y- and z-direction respectively. In developing numerical solutions it is usual to relate the eddy diffusivity K_y for the vertical flux to the eddy viscosity ν_T via a relation of the form

$$K_y=\nu_T/Pr_t$$

where Pr_t is the turbulent Prandtl or Schmidt number. However, no equivalent formulation exists for the diffusivity K_z of the lateral flux and it is known that the turbulent Prandtl number must be a function of the height from the solid surface and another empirical relation is needed[1,2]. Further, combined with equations (2a, b), equation (1) becomes parabolic while the turbulent diffusion shows the wave-like characteristics[3].

Another approach is to use so-called second-order closure models. Bradshaw and Ferriss[4] assumed that statistical properties of the temperature fluctuation field can be expressed as empirical functions of the heat flux and shear stress profile and modelled the transport equation for the mean square of temperature fluctuations adopting the turbulent bulk-convection velocity representation proposed by Townsend[5]. Lewellen and Teske[6] developed a method for calculating turbulent diffusion in the planetary boundary layer using second-order closure approach and showed that the resulting partial differential equation for the turbulent mass flux has a hyperbolic character for early times, when the plume scale is small compared with the ambient turbulent scale, with a smooth transition to a parabolic, gradient diffusion-type character when the plume scale is large. Gosman et al.[7] obtained fairly good results using Rodi's[3] algebraic equation turbulence model.

The present contribution adopts the same general approach as the above second-order closure models but in a slightly different way. Pressure scrambling terms are modelled following Launder[9] but the constants are assumed to be functions of plume width. Instead of taking conventional gradient diffusion or turbulent bulk-convection velocity model, turbulent transport terms are assumed to be functions of plume width and height and their inter-relationships are formulated according to the measurements of Nakayama and Bradshaw[10].

Ⅱ. Turbulence Modelling

Boundary layer approximations of transport equations for mean fluxes, $\overline{vc}$ and $\overline{wc}$, become, neglecting molecular effects,

$$U\frac{\partial\overline{vc}}{\partial x}+V\frac{\partial\overline{vc}}{\partial y}+W\frac{\partial\overline{vc}}{\partial z}=-\overline{v^2}\frac{\partial C}{\partial y}-\overline{vc}\frac{\partial V}{\partial y}+\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial y}}-\frac{\partial}{\partial y}\left(\frac{\overline{p'c}}{\rho}+\overline{v^2c}\right)-\frac{\partial\overline{vwc}}{\partial z} \tag{3a}$$

and

$$U\frac{\partial\overline{wc}}{\partial x}+V\frac{\partial\overline{wc}}{\partial y}+W\frac{\partial\overline{wc}}{\partial z}=-\overline{w^2}\frac{\partial C}{\partial z}-\overline{vc}\frac{\partial W}{\partial y}+\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial z}}-\frac{\partial\overline{vwc}}{\partial y}-\frac{\partial}{\partial z}\left(\frac{\overline{p'c}}{\rho}+\overline{w^2c}\right) \tag{3b}$$

In equations (3a, b) generation terms, $-\overline{v^2}\frac{\partial C}{\partial y}$, etc., needs no further modelling. The behaviour of the correlation $\overline{p'\frac{\partial c}{\partial y}}$ has been discussed by Launder[9]. He argues that like its counterpart in the Reynolds stress transport equation it contains two parts (three in a buoyant flow) corresponding to the two parts of the source term in the Poisson equation for the pressure fluctuations p'. However the lack of sufficient experimental measurements on the contribution due to the mean strain makes it difficult to model properly and, more over, in the neutral boundary layer the generation of mean fluxes due to the mean strain which is generally of the same form as those frequently suggested for the contribution to the pressure scrambling terms due to the mean strain is negligible. Hence it is simply neglected and only the contribution due to the turbulence is considered.

The most widely used form for the contribution to the pressure scrambling terms due to the turbulence is and so $\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial y}}$ could be approximated by

$$\frac{1}{\rho}\overline{p^1\frac{\partial c}{\partial y}}=-c_{1c}\frac{2\varepsilon}{\overline{q^2}}\overline{vc}, \tag{4}$$

where $\overline{q^2}/2$ and ε represent the turbulent kinetic energy and its dissipation rate, respectively. c_{1c} is a constant whose value is about 3.4[9].

Instead of adopting eq. (4) directly, we take a rather simplified form. In a boundary layer outside the viscous sublayer

$$\overline{q^2}/2\simeq-3\overline{uv}$$

and

$$\varepsilon=(-\overline{uv})^{3/2}/l,$$

where l is a mixing length. Thus eq. (4) could be reduced to

$$\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial y}}=-c_{fy}\frac{\sqrt{-\overline{uv}}}{l}\overline{vc}, \tag{5}$$

where c_{fy} is a constant whose value is about 1.

Eq. (5) could be derived in a different way. Applying the local-equilibrium assumption to eq. (3a) we get

$$\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial y}}\simeq\overline{v^2}\frac{\partial C}{\partial y}$$

The definition of the mixing length l_c for C says

$$\frac{\partial C}{\partial y}=\frac{-\overline{vc}}{(-\overline{uv})^{1/2}l_c}$$

Thus

$$\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial y}}\simeq\overline{v^2}\frac{\partial C}{\partial y}=-\frac{\overline{v^2}}{(-\overline{uv})^{1/2}}\frac{\overline{vc}}{l_c}$$
$$=-\frac{l}{l_c}\frac{\overline{v^2}}{(-\overline{uv})^{1/2}}\frac{\overline{vc}}{l} \tag{6}$$

In a boundary layer

$$\overline{v^2}\simeq-\overline{uv}$$

and, if the plume scale is large enough so that the local-equilibrium condition can be applied, we could assume

$$l_c\simeq l$$

Hence we get eq. (5) again.

At the early stage of the plume when the plume scale is small, however, it is difficult to assume that l_c will be of the same order of l, which means that c_{1c} or c_{fy} can not be a constant but a function of l and l_c, i.e.,

$$c_{fy}=f_1\left(\frac{l_c}{H},\ \frac{l}{H}\right) \tag{7}$$

where H is a plume source height from the ground. When the plume scale is small to cover only a small portion of the boundary layer, l will be nearly constant and l/H could be dropped from eq. (7). When the plume scale is large to cover a significant part of the boundary layer, l_c will be of the same order of l and l/H could be dropped again. In other words c_{fy} is more closely related to l_c/H than to l/H and to the first approximation the terms containing l/H could be neglected in the eq. (7). If we assume further that l_c is directly related to the plume length scale l_p when the plume scale is small, we can write

$$c_{fy}=f(l_p/H), \tag{8}$$

since c_{fy} approaches to a constant and becomes independent of l_c and l_p when the plume scale is large. Equation (5) and (6) say that c_{fy} must be inversely proportional to l_c when the plume scale is small. The simplest funtional form satisfying the above conditions seems to be

$$c_{fy}=\frac{c_y}{l_p/H}+d_y \tag{9}$$

where c_{fz} and d_y are constants. d_y must be of order 1.

Similar arguements can be applied to another pressure scrambling term $\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial z}}$, which leads to

$$\frac{1}{\rho}\overline{p'\frac{\partial c}{\partial z}}=-c_{fz}\frac{\sqrt{-\overline{uv}}}{l}\overline{wc} \tag{10}$$

and

$$c_{fz}=\frac{c_2}{l_p/H}+d_z$$

The constants c_y, d_y, c_z, and d_z have been determined by comparing the numerical results with the experimental results of Nakayama and Bradshaw[10]. Their values are taken to be 1.65, 1.0, 1.98, and 0.5, respectively.

One of the widely accepted models for the triple products $\overline{v^2c}$, $\overline{vwc}$, etc. may be a so-called gradient diffusion model like

$$\overline{v^2c}=\frac{\partial\overline{vc}}{\partial y}\sqrt{-\overline{uv}}\; l_p f_2\left(\frac{y}{H},\ \frac{z}{H},\ \frac{l_p}{H}\right)$$

Though it has a merit that it prevents excessive gradients in the species flux, it makes the governing equations parabolic. There is no reason that a gradient diffusion model will be applied well to the second-order closure models while eddy diffusivity models for the mean concentration do not work satisfactorily.

Another approach is to put into formular directly. Nakayama and Bradshaw[11] suggested formular like

$$\overline{v^2c}=\sqrt{(\overline{vc}^2+\overline{wc}^2)(-\overline{uv})}\,f_3\left(\frac{y}{H},\ \frac{z}{H},\ \frac{l_p}{H}\right)$$

without giving an explicit expression of f_3. But their experimental results[10] show that $\overline{v^2c}$ is not zero at the point of maximum concentration were $\overline{vc}$ and $\overline{wc}$ must vanish. $\overline{c^2}$ may be used instead of $\sqrt{(\overline{vc}^2+\overline{wc}^2)}$ in the above formular, which requires another equation for $\overline{c^2}$. To avoid solving an equation for $\overline{c^2}$, the maximum concentration C_{max} is taken instead of $\overline{c^2}$. Hence the expression will be of the form

$$\overline{v^2c}=C_{max}(-\overline{uv})g_1\left(\frac{y}{H},\ \frac{z}{H},\ \frac{l_p}{H},\ \frac{y_{max}}{H},\ \frac{z_{max}}{H}\right) \tag{12}$$

where y_{max} and z_{max} are coordinates of the point of maximum concentration. Last two non-dimesional parameters, y_{max}/H and z_{max}/H, in eq. (12) are added to give more generality to the expression. To make the work simpler it was assumed that the function g_1 can be separable, i.e.,

$$\frac{\overline{v^2c}}{(-\overline{uv})C_{max}}=Y_1\left(\frac{y}{H},\ \frac{l_p}{H},\ \frac{y_{max}}{H}\right)\times Z_1\left(\frac{z}{H},\ \frac{l_p}{H},\ \frac{z_{max}}{H}\right)$$

The experimental results of Nakayama and Bradshaw[10] have been used to get explicit expressions of Y_1 and Z_1 and corresponding ones for $\overline{w^2c}$ and $\overline{vwc}$. The formulae are

$$\frac{\overline{v^2c}}{(-\overline{uv})C_{max}}=0.25\frac{l_p}{H}\frac{y}{l_p}\left(\frac{y-y_{max}}{l_p}-0.25\right)\times\exp\left(-3.22\left(\frac{y-y_{max}}{l_p}-0.25\right)^2-1.93\left(\frac{z-z_{max}}{l_p}\right)^2\right), \tag{13}$$

$$\frac{\overline{w^2c}}{(-\overline{uv})C_{max}}=0.20\frac{l_p}{H}\left(\frac{(z-z_{max})^2}{l_p^2}-0.04\right)\times\exp\left(-2.77\left(\frac{y-y_{max}}{l_p}\right)^2-1.11\left(\frac{z-z_{max}}{l_p}\right)^2\right) \tag{14}$$

and

$$\overline{vwc}=0. \tag{15}$$

The pressure transport term $\overline{p'c}/\rho$ is simply neglected. This is equivalent to assume that in the equations âbove the pressure transport term $\overline{p'c}/\rho$ is contained in the triple product terms implicitly, i.e.,

$$\frac{\overline{v^2c}+\frac{\overline{p'c}}{\rho}}{(-\overline{uv})C_{max}}=0.25\frac{l_p}{H}\frac{y}{l_p}\left(\frac{y-y_{max}}{l_p}-0.25\right)\times\exp\left(-3.22\left(\frac{y-y_{max}}{l_p}-0.25\right)^2-1.93\left(\frac{z-z_{max}}{l_p}\right)^2\right) \tag{13'}$$

and

$$\frac{\overline{w^2c}+\frac{\overline{p'c}}{\rho}}{(-\overline{uv})C_{max}}=0.20\frac{l_p}{H}\left(\left(\frac{z-z_{max}}{l_p}\right)^2-0.04\right)\times\exp\left(-2.77\left(\frac{y-y_{max}}{l_p}\right)^2-1.11\left(\frac{z-z_{max}}{l_p}\right)^2\right) \tag{14'}$$

There are various ways to define the plume length scale l_p. In this study it is defined as twice of the vartical distance from the point of maximum concentration to the point where the concentration is a half of maximum concentration in the plane of symmetry. At the initial stage of the plume where the plume is almost symmetric this is same as the half-width of the plume defined as the vertical distance between two points whose concentration is a half of maximum concentration, but they deviate from each other as the plume goes downstream and the point of maximum concentration approaches the ground.

III. Method of Solution

The "Hopscotch" algorithm[12] is used to solve the set of governing equations. It has an advantage in ease of programming and running speed comparing to the other powerful methods such as the alternating-diretion implicit method and Keller and Cebeci's box method.

The boundary conditions on the ground is the "impermeable" one. In order to avoid calculations in the viscous sublayer for a smooth wall or in the roughness-influenced region for a rough wall, a height of 20 times roughness height or viscous length scale ν/u_τ from the wall is taken as the effective ground. There $\partial C/\partial y=\overline{vc}=0$.

Conditions at infinity are replaced by conditions at finite distances from the plume centre line where $C=\overline{vc}=\overline{wc}=0$.

Before the plume reaches the ground, this condition is used on all four sides of the calculation domain. When the plume nears the ground the condition here is replaced by the impermeable condition above.

IV. Results and Discussion

For the calculations presented here, data on turbulence are given according to the experimental results of Nakayama and Bradshaw[10] who measured in a simulated neutral atmospheric boundary layer. They are shown in Fig. 1, 2, and 3. They obtained the value of the friction velocity u_τ from the mean velocity profile, but it shows a slight inconsitency with the measurements of the shear stress. However we followed their measurements without correction. The values of the mixing lengths are calculated from the mean velocity and shear stress profile and might be erroneous at the outer edge of the boundary layer ($y/H>2.5$)

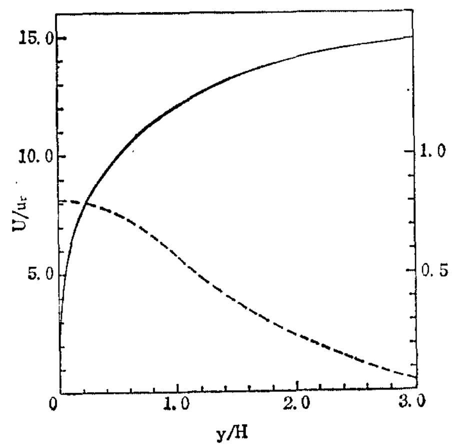


Fig. 1 Velocity and shear stress across a simulated neutral atmospheric boundary layer (from Nakayama and Bradshaw[10]), **—mean velocity; ···Reynolds stress**

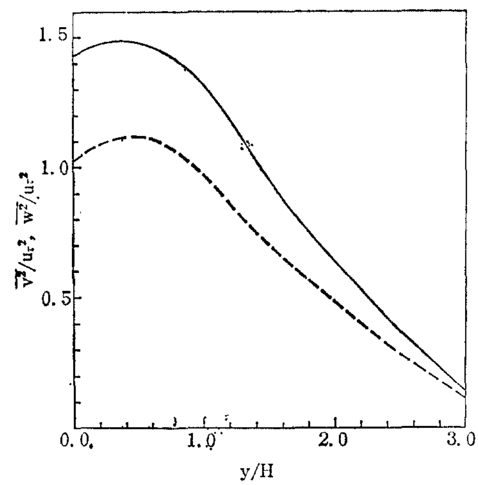


Fig. 2 Turbulence intensity profiles across a simulated neutral atmospheric boundary layer (from Nakayama and Bradshaw[10]), $-\overline{w^2}/u_\tau^2$; $\cdots\overline{v^2}/u_\tau^2$

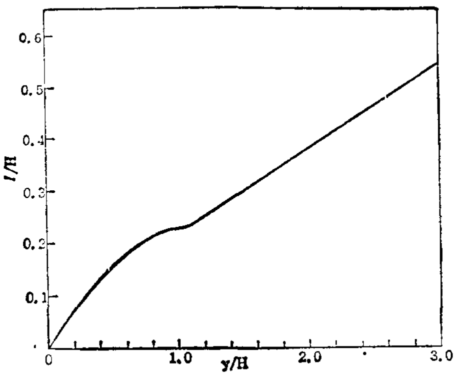


Fig. 3 Variation of mixing length across a simulated neutral atmospheric boundary layer (calculated from the experimental data of Nakayama and Bradshaw[10])

as both the gradient of the mean velocity and the shear stress are too small.

Initial concnetration of the plume is assumed to be Gaussian and the mean fluxes are set to zero. The numerical results show that it can be assumed that the point source is located at the upstream and in the following discussion the streamwise coordinate is measured from that point source.

Fig. 4 shows the variation of the plume length scale l_p of the plume. The results are in fairly good agreement with Nakayama and Bradshaw's[10] experimental results. Unexpectedly the plume length scale l_p increases almost linearly as the plume goes downstream while the vertical and lateral half-width of the plume, l_{py} and l_{pz}, defined as the distances between the points whose concentration is a half of the maximum concentration* increase a little slowly. For early times when the plume scale is small the turbulent dispersion is wave-like and the plume length scale will increase linearly. In the downstream where the plume scale is large the turbulent dispersion becomes

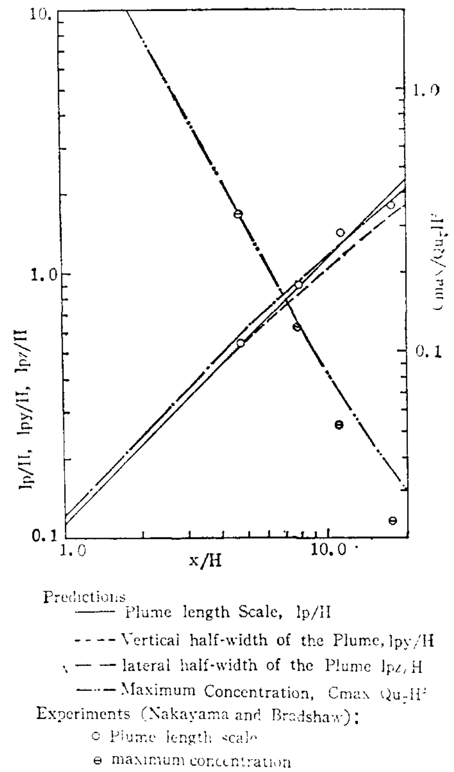


Fig. 4 Variation of width and maximum concentration of the plume

more parabolic and the half-widths of the plume will increas directly as the square root of the downstream distance, but the point of maximum concentration nears the ground, which helps the plume length scale increase more rapidly.

The ratio of the lateral halfwidth to the vertical half-width, l_{pz}/l_{py}, is about 1.1. This means that the ratio of the eddy diffusivity, K_z/K_y, is about 1.2, the value frequently suggested by various authors[9].

The variation of the maximum concentration is also shown in Fig. 4. At the early times when the plume scale is small it varies like

$$\frac{C_{max}}{Q u_\tau H^2} = 6.0 \left(\frac{x}{H} \right)^{-1.85}$$

* When the concentration at the effective ground is greater than the half of the maximum concentration, the vertical half-width is defined as the distance from the effective ground.

Table. 1

x/H	Experimental			Predicted		
	l_p/H (A)	$C_{max}/Qu_\tau H^2$ (B)	A^2B	l_p/H (C)	$C_{max}/Qu_\tau H^2$ (D)	C^2D
4.7	0.54	0.33	0.096	0.54	0.33	0.096
7.9	0.90	0.125	0.101	0.90	0.13	0.105
11.3	1.4	0.053	0.104	1.3	0.07	0.118
17.8	1.8	0.023	0.075	2.0	0.035	0.140

where Q is the point source strength. In the downstream predicted decreasing rate of the maximum concentration drops slightly, while the experimental results do not. This may be due to the loss of heat by various reasons such as radiation and conduction through the wall in the experiment. If the concentration profile is assumed to be self-preserving, it can be expected that $C_{max}l_p^2$ will remain nearly constant. Table 1 compares the values of $(l_p/H)^2C_{max}/Qu_\tau H^2$. In the experimental results it drops rapidly at $x/H=17.8$, while the predicted value increases monotonically. The latter is more reasonable. As the plume goes downstream the concentration profile becomes more unsymmetric (Fig. 3) and $l_p^2C_{max}$ will increase.

Predicted iso-concentration contours and concentration profiles in the plane of symmetry are shown in Fig. 6 and 5, respectively, and again show fairly good agreement with the experiment. At the early times the concentration profile is symmetric, but as the plume goes downstream it becomes more unsymmetric and the point of the maximum concentration approaches the ground.

V. Conclusion

A method for computing turbulent diffusion based on second-order closure, which appears to be in general agreement with the experiments, has been presented. The dissipation of the mean scalar flux due to the pressure

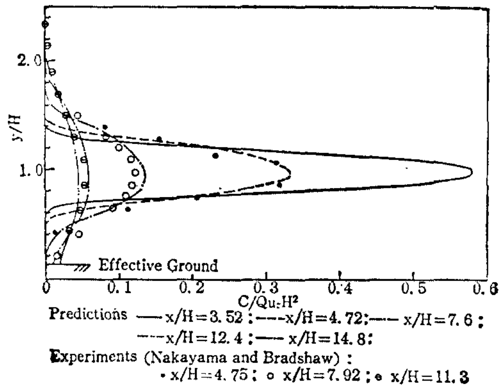


Fig. 5 Variation of the concentration profile in the plane of symmetry

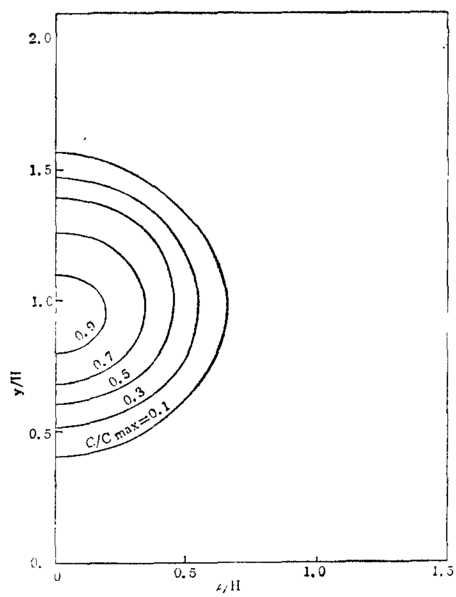
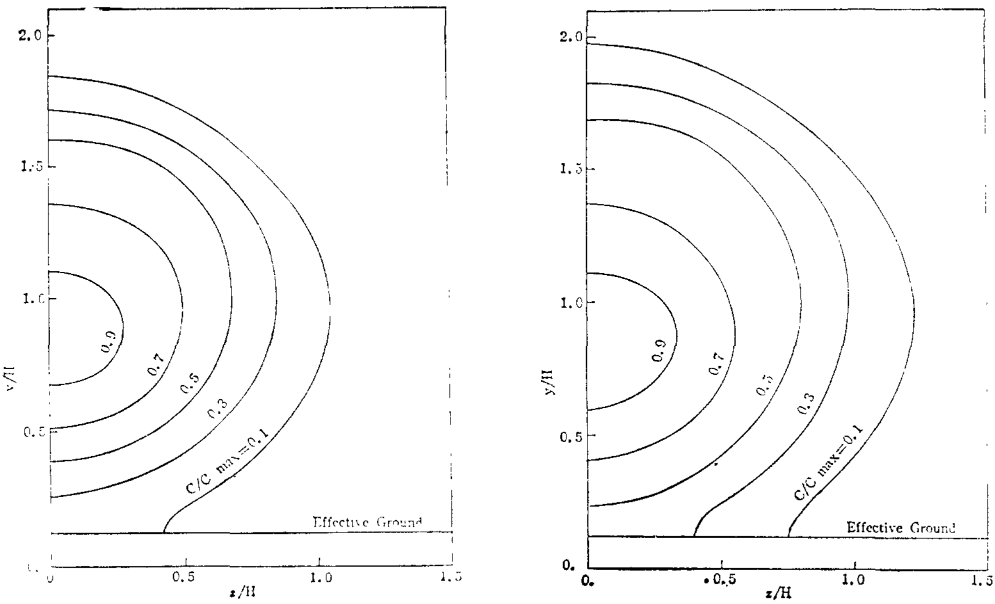


Fig. 6 (a) For legend see page 76



(b) (c)

Fig. 6 Predicted iso-concentration contours of the plume at (a) $x/H=7.6$, (b) $x/H=12.4$, and (c) $x/H=14.8$

scrambling is assumed to be inversely proportional to the plume length scale when the plume scale is small.

In a neutral turbulent boundary layer the plume length scale defined as the distance from the point of maximum concentration to the point whose concentration is a half of the maximum concentration appears to increase almost linearly as the plume goes downstream, while the plume half-widths increase slightly slowly. The maximum concentation varies as -1.85 power of the streamwise distance from the point source when the plume scale is small.

This work was carried out when the author was at Imperial College. The author gives deep thanks to Prof. P. Bradshaw for his kind advice and to the British Council whose fellowship helped him study in England.

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