

A one-dimensional model based on k- ϵ taking into account the change in basic atmospheric flow with height and stability

J. Servert¹, J. Lumbreras², M. E. Rodríguez² & A. Crespo¹

¹*Department of energy and fluid mechanics, Universidad Politécnica de Madrid (UPM), Spain*

²*Department of Chemical and Environmental Engineering, UPM, Spain*

Abstract

A one-dimensional model has been developed to evaluate the ambient air quality standards due to the discharge of pollutants through a stack. This model has been applied to a tire thermolysis plant in Ardoncino, Leon, Spain. The plume centerline is evaluated by mean of the fluid mechanics conservation equations and a gaussian-distribution hypothesis is made to estimate the flow magnitudes in radial direction. The mass entrained in the plume is calculated with two different models, one based on the difference of velocities (Escudier [8]) and the other on the turbulent viscosity (Tamanini [19]). The model takes into account the following effects: ambient turbulence, turbulent kinetic energy and its dissipation, change in basic atmospheric flow with height and stability. Different averages are made: weekly, monthly and annual averages, taking into account the different wind directions, stability and temperature.

1. Introduction

The aim of atmospheric modelling is to analyse the impact of some pollutants in a specific study area. The goal is usually the study and modelling of atmospheric-pollutant physic-chemicals processes with mathematical models, taking into account the specific characteristics of the analysed environment.

The description of pollutant concentration related with time is more accurate when diffusion models are fitted to a meteorological model. The coordinated measures of relevant parameters from each model will be input data for model consistent by itself. Prediction of the pollutants diffusion from a stack for tens of

kilometres could be tackled with different approaches of varying complexity. For the case of 2-4 kilometres can be used a simply one-dimensional model based on a cross-section distribution hypothesis (in this case, gaussian distribution).

Pollutants diffusion depends on atmospheric characteristics (wind, vertical stability, precipitation, fog, etc.). Therefore, every diffusion study should include the observation or simulation of strictly atmospheric variables. To estimate pollutant diffusion in periods of approximately between 12&24 hours, it must be considered the atmospheric development. The model described in this paper can be used to evaluate concentration averages for long periods of time (weeks, months, a year, etc.). To do so, the model evaluates plumes for each possible atmospheric situation assuming it to be cuasi-stationary and after that, averages each result with the probability of the associated atmospheric conditions to obtain the mean concentrations. Variation in atmospheric magnitudes (temperature, wind speed and direction, atmospheric stability) for day and night is considered.

2. Object of this one-dimensional model

To approximately predict the diffusion of pollutants from a stack, there are different approaches and models. The most simple is the use of regression formula adjusted from experiments to evaluate concentration of pollutants as in Kunkel [12], Britter [2], Hanna [10] and Briggs [1]. Another one is the use of gaussian plume models, that have been extensively used as in Eltgroth [5], Hanna [10], Irwin [11] and Cramer [4]. The last option is integrating the fluid mechanics equations in surfaces normal to the mean flow line and an entrainment model Ooms [13], Ermark [6], Cox [3].

The model presented in this work is based on integrating the 3-D equations in perpendicular planes, considering the different source terms and the influence of the distribution profiles over them. On the other hand, different entrainment models have been analysed and two have been selected: a classical one, and another calculated by the turbulent viscosity that is estimated from the k- ϵ model. The model evaluates the turbulent kinetic energy in the plume and its dissipation rate. The model has retained the evolution of the atmosphere with height and the effect over the conservation equations.

3. Flow equations

The one-dimensional conservation equations of mass, momentum, energy, pollutant concentration, turbulent kinetic energy, (k) and dissipation rate of turbulent kinetic energy, (ϵ) are obtained from the classical three-dimension equations for turbulent flow. The magnitudes k and ϵ are needed to close the turbulent transport terms. These equations can be written, for the stationary case, in the general form of eqn (1). In this equation, ϕ can be equal to 1 or any component of the velocity (v_i) or total enthalpy (h) or pollutant mass fraction (Y) or turbulent kinetic energy (k) or also dissipation rate of the turbulent kinetic energy (ϵ). These variables are Favre averaged but density, ρ , is time averaged.

$$\frac{\partial}{\partial x_i} (\rho v_i \phi - \Gamma_{\phi_i}) = S_{\phi} \quad (1)$$

The diffusion vector is expressed as eqn (2) for the scalar variables and in eqn (3) it is expressed for the turbulent Reynolds stresses, where μ_t is the turbulent dynamic viscosity [eqn (4)], and σ_{ϕ} is the turbulent Prandtl number for the variable ϕ . C_{μ} is the classical coefficient of the k- ϵ model, that usually takes the value of 0.09

$$\Gamma_{\phi_i} = \frac{\mu_t}{\sigma_{\phi}} \frac{\partial \phi}{\partial x_i} \quad (2)$$

$$\tau_{ij} = \mu_t \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\mu_t \frac{\partial v_k}{\partial x_k} + \rho k \right) \quad (3)$$

$$\mu_t = C_{\mu} \cdot \rho \left(\frac{k^2}{\epsilon} \right) \quad (4)$$

The source terms include buoyancy effects in the vertical momentum equation, and production and dissipation terms in the equation for k and ϵ . The model is completed with the Law of Perfect Gases, where pressure is assumed to be equal to the ambient pressure.

The stack discharges into a non-uniform atmosphere flow at ambient pressure. Flow magnitudes change vertically in relation with the laws that show the changing of flow magnitudes in the atmospheric boundary layer. In the plume, the existence of self-similar profiles in planes normal to a central line is assumed. The central line is assumed to be contained in a plane normal to the ground. It is also assumed, that, in planes normal to the central line, the perturbations of all dependent variables are greater at the central line itself, and decays tending to zero for high enough values of the radial distance (r), to the central line. For all the dependent variables in eqn (1), it is assumed that there are self-similar profiles of the form of eqn (5) where the subindex a means ambient, ϕ is the azimuthal angle; ψ_{ϕ} and R_{ϕ} satisfy the normalisation conditions of eqn (6).

$$\phi - \phi_a = (\phi_c - \phi_a) \psi_{\phi} \left(\frac{r}{R_{\phi}}, \varphi \right) \quad (5)$$

$$\int_0^{2\pi} \int_0^{\infty} \psi_{\phi} r dr d\varphi = \pi R_{\phi}^2, \psi_{\phi}(0, \varphi) = 1 \quad (6)$$

R_{ϕ} and ϕ_c are functions of the coordinate along the central line (s) to be calculated with the 1-D model. A discussion of possible profiles, the effect of the central line curvature and the effect of buoyancy can be found in Servert [17].

The conservation equations of flow magnitude are obtained from the 3-D equations by integrating them in cross sections (Servert [17]) and defining two spatial averages shown in eqn (7-8).

$$m(\langle \phi \rangle - \phi_a) = \lim_{A \rightarrow \infty} \int_A (\rho u (\phi - \phi_a)) dA; \quad (7)$$

$$m(1 - m_a) = \lim_{A \rightarrow \infty} \int_A (\rho u - \rho_a v_a \cos \theta) dA, \quad m_a = \frac{\rho_a v_a \cos \theta}{\rho_m \langle u \rangle} \quad (8)$$

where A is contained in the plane normal to the central line, u is the velocity component normal to A, θ is the angle of u with the horizontal and ρ_m is an average density that satisfies the equation of state for the averaged magnitudes.

The general 1-D equation is eqn (9) where $\Delta \Sigma_\phi$ is the increment of the source term and m'_0 is the entrained mass per unit of time and length. This equation applies to the same variables as eqn (1).

$$\frac{d(m \langle \phi \rangle)}{ds} = m'_0 \phi_a + \Delta \Sigma_\phi + m_a \frac{d\phi_a}{dS} \quad (9)$$

4. Basic flow

The incident flow is due to the surface layer of the atmospheric boundary layer in flat and uniform ground. Flow properties are described with eqn (10)- (15), most of them are based on [14] as functions of height, "y", surface roughness of the ground, "z₀", turbulent friction velocity, "u*", and the Monin-Obukhov length (related to atmospheric stability), L. θ is the potential temperature and θ_a is related with temperature by eqn (14). When L < 0 there is an unstable atmosphere [eqn (16)- (19)], however when L > 0, the atmosphere is stable [eqn (20)- (23)]. For the case of a neutral atmosphere, the Monin-Obukhov length is equal to infinity. For every L value eqn (24) is used.

$$u_a = 2.5 u^* [\log(y/z_0) - \Phi_m] \quad (10)$$

$$k_a = C_\mu^{-0.5} (u^*)^2 \phi_k \quad (11)$$

$$\varepsilon_a = 2.5 (u^*)^3 (\phi_\varepsilon / y) \quad (12)$$

$$\theta_a = \theta(y=0) + 2.5 \cdot \theta^* [\log(y/z_0) - \Phi_h] \quad (13)$$

$$\theta_a = T(P/P(y=0))^{(\gamma/(\gamma-1))} \quad (14)$$

$$\theta^* = (u^*)^2 T_a / (0.4 g \cdot L) \quad (15)$$

$$\Phi_m = \log \left[\frac{(1 + \alpha_1^2) \cdot (1 + \alpha_1^2)}{8} \right] - \text{atan}(\alpha_1) + \pi/2, \quad \alpha_1 = 1/\phi_m \quad (16)$$

$$\phi_m = (1 - 16y/L)^{-0.25} \quad (17)$$

$$\phi_\varepsilon = 1 - y/L \quad (18)$$

$$\Phi_h = 2 \log \frac{1 + (1 - 16y/L)^{0.5}}{2} \quad (19)$$

$$\Phi_m = 1 - \phi_m \quad (20)$$

$$\phi_m = 1 + 5y/L \quad (21)$$

$$\phi_\varepsilon = \left[1 + 2.5(y/L)^{0.6} \right]^{3/2} \quad (22)$$

$$\Phi_h = \Phi_m \quad (23)$$

$$\phi_k = (\phi_\varepsilon / \phi_m)^{0.5} \quad (24)$$

$\Phi_m, \Phi_h, \phi_m, \phi_\varepsilon, \phi_k$ are functions that represent the effect of atmospheric stability.

5. Mass entrainment models.

To estimate the mass entrainment, two classical models are used. In the first one three contributions are taken into account. First, it is considered that in the area close to the stack exit, gas velocity is much higher than that of the wind and therefore it is assumed that entrainment is similar to the one which would be produced by a turbulent free jet [eqn (25)].

$$\dot{m}'_{01} = \alpha_1 \rho_a |u - u_v \cos \theta| 2\pi b \quad (25)$$

where $\alpha_1=0.057$ is a semiempiric coefficient, ρ_a is outside fluid density, $u_v \cos \theta$ is the wind velocity component in the plume direction and b is the radius that would have a uniform jet with the same spatial averaged values as the one considered.

Second, in areas far away from the exit, jet velocity approaches wind velocity. In this case, the model identifies the plume with a hot cylinder inside a colder atmosphere. Entrainment will be calculated with eqn (26), where $\alpha_2=0.5$ is the entrainment coefficient for a hot cylinder.

$$\dot{m}'_{02} = \alpha_2 \rho_a u_v 2\pi b |\sin \theta| \cos \theta \quad (26)$$

Third, atmospheric turbulence also causes air entrainment to the plume. This phenomenon is shown in eqn (27) where $\alpha_3=1$ is a entrainment coefficient and u' is the turbulent entrainment velocity [eqn (28)].

$$\dot{m}'_{03} = \alpha_3 \rho_a u' 2\pi b \quad (27)$$

$$u' = \sqrt[3]{\varepsilon b} \quad (28)$$

Total entrainment could be aggregated in eqn (29) where the average of densities is due to [16]. $\cos\theta$ is included to neglect m'_{02} at the part of the plume closest to the stack.

$$m'_0 = 2\pi b \rho_a \sqrt{\frac{\rho_m}{\rho_a}} \left[\alpha_1 |u - u_v \cos\theta| + \alpha_2 u_v |\sin\theta| \cos\theta + \alpha_3 u' \right] \quad (29)$$

The second model is based on Tamanini [19] and supposes that the entrainment can be obtained from eqn (30), deduced by a laminar jet entrainment analogy. Laminar transport is ignored in comparison with turbulent transport. Turbulent viscosity, " μ_t ", is obtained from the classic k- ϵ method [eqn (31)] directly applied to the averaged values. And C_m takes the value of 19 as discussed in [17]

$$m'_0 = C_m \pi \mu_t \quad (30)$$

$$\mu_t = C_\mu (\rho_a \rho)^{1/2} \frac{\langle k \rangle}{\langle \epsilon \rangle} \quad (31)$$

6. Source terms

A detailed description of the source terms can be found in [17], specially the source term in the k equation. As a summary for this model, the source term for the momentum equation for a Gaussian profile is shown in eqn (32) where g is the gravity. The turbulent kinetic energy has three terms. The first one takes into account the mechanical production of k, it can be simplified to eqn (33) where the β_v factor takes into account the gaussian profile, and evolves from 4/3 to one as the velocity approaches to the ambient one. The floatability term is shown in eqn (34) where density fluctuations are supposed to be proportional to the difference between air and plume densities. The third term is the difference between the ambient and plume dissipation rate of k.

$$\Delta\Sigma_{vz} = (\rho_a - \rho_m) g \pi b^2 \quad (32)$$

$$\Delta\Sigma_{k1} = \beta_v m_0 0.5 (\langle v \rangle - v_a)^2 \quad (33)$$

$$\Delta\Sigma_{k2} = \frac{g}{\sigma_h} \left(\frac{\mu_a}{\rho_m} \cdot \frac{d\rho_m}{ds} - \frac{\mu_a}{\rho_a} \cdot \frac{d\rho_a}{ds} \right) \quad (34)$$

7. Comparison of results with classical models.

The results are compared with a classical model considering the following hypothesis:

1. The pollutant dispersion is a stable process and chemical pollutants are non-reactive.
2. The cross wind is stable.

3. The pollutants are horizontally and vertically dispersed according to a gaussian profile. The axial pollutant dispersion is caused by wind convection whereas lateral dispersion is caused by turbulent diffusion.
4. The surface earth layer is flat and reflectant so, every pollutant which contacts with the ground, except settling particle matter, will bounce to the air.

With those hypothesis the temporal average pollutant concentrations in any (x,y,z) plume point is shown in eqn (35). And ground concentration is eqn (36) where Q is the output stack pollutant flow, σ_y y σ_z are vertical and horizontal dispersion rates that show the downstream diffusion. To estimate them, Briggs values [15] for high discharges in open field are used as table 1 shows.

$$c(x, y, z) = \left[\frac{Q_P}{2\pi U \sigma_y \sigma_z} \right] \exp\left\{-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right\} \left\{ \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] \right\} \quad (35)$$

$$c(x, y, 0) = \left[\frac{Q_P}{\pi U \sigma_y \sigma_z} \right] \exp\left\{-\frac{1}{2}\left[\left(\frac{y}{\sigma_y}\right)^2 + \left(\frac{H}{\sigma_z}\right)^2\right]\right\} \quad (36)$$

On the other hand, the dispersion in the horizontal direction normal to the wind has been increased in both models according to Slade's work and its experimental validation by Ermak [7] for LNG dispersion, it is estimated that σ_y is increased by zigzagging effect in the period t_{av} , in a rate [eqn (37)] where $\tau_0=10$ s. This rate has an error of less than 10% respect Peterson values.

$$\sigma = \left[\frac{t_{av} + \tau_0 e^{-t_{av}/\tau_0}}{\tau_0} \right]^{0.2} \quad (37)$$

This is a rough approach. According with [18], to estimate the concentration under ideal conditions, where the ground is uniform and meteorological conditions are constant, the maximum ground concentration error is between 10 and 20% of the calculated value for a ground source and between 20 and 40% of the estimated value for an elevated one. The model used for validation is this classical gaussian plume model but improved because the centre line is the one calculated with this model instead of a straight line. So the concentration fault is expected to be smaller.

8. Atmospheric characterisation

To estimate σ_y y σ_z and the Monin-Obukhov length, it is necessary to determine basic flow magnitudes. Pasquill [15] categories are used and their equivalence with the Golder ones [9]. For ground roughness z_0 value is estimated, equal to 0.05 m. Categories are resumed in table 2.

Table 1: Briggs $\sigma_y(x)$ y $\sigma_z(x)$ values for high discharges, $0.1 \leq x \leq 10$ km.

	Stability	σ_y	σ_z
Open field	A	$0.22x(1+0.1x)^{-1/2}$	$0.20x$
	B	$0.16x(1+0.1x)^{-1/2}$	$0.12x$
	E	$0.11x(1+0.1x)^{-1/2}$	$0.08x(1+0.2x)^{-1/2}$
	D	$0.08x(1+0.1x)^{-1/2}$	$0.06x(1+1.5x)^{-1/2}$
	E	$0.06x(1+0.1x)^{-1/2}$	$0.03x(1+0.3x)^{-1}$
	F	$0.04x(1+0.1x)^{-1/2}$	$0.016x(1+0.3x)^{-1}$
Urban areas	A-B	$0.32x(1+0.4x)^{-1/2}$	$0.24x(1+0.1x)^{-1/2}$
	C	$0.22x(1+0.4x)^{-1/2}$	$0.20x$
	D	$0.16x(1+0.4x)^{-1/2}$	$0.14x(1+0.3x)^{-1/2}$
	E-F	$0.11x(1+0.4x)^{-1/2}$	$0.08x(1+0.15x)^{-1/2}$

Table 2: Stability categories depending on wind velocity, insolation and sky state

Wind velocity (m/seg)	Insolation			Sky	
	High	Moderate	Low	Slightly overcast	Overcast
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Note: for A-B similar values, the average value will be taken

9. Results of the application to a tire thermolysis plant

The model has been applied to a tire thermolysis plant in Ardoncino, León (Spain). Discharge characteristics are shown in table 3. As an example, figures 1-3, display the results for a typical spring day. They show the centreline evolution and the maximum concentrations of pollutant within the nearest 4 km² to the plant stack. It is possible to conclude that anywhere regulations are fulfilled.

Table 3: Discharge characteristics

Parameter	Value
Gas flow	$55549 \text{ m}^3/\text{h} = 34232 \text{ Nm}^3/\text{h} = 11.79 \text{ kg/s}$
Discharge temperature	$170 \text{ }^\circ\text{C} = 443 \text{ K}$
Stack height	25 m
Stack diameter	1 m
Particle matter concentration	$9.6 \text{ mg/Nm}^3 = 5.916 \text{ mg/m}^3$
SO ₂ concentration	$30 \text{ mg/Nm}^3 = 18.488 \text{ mg/m}^3$
CO concentration	$49.5 \text{ ppm} = 61,875 \text{ mg/Nm}^3$
NO _x	$78.9 \text{ ppm} = 116.941 \text{ mg/Nm}^3$

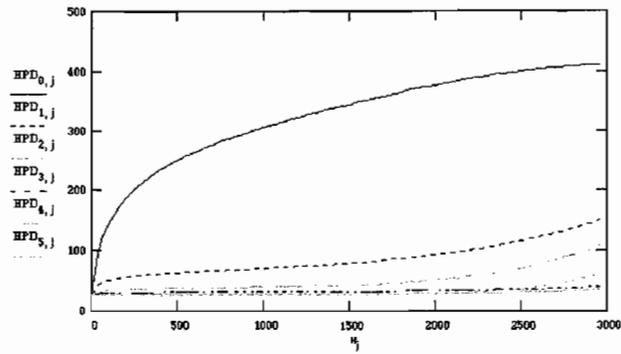


Figure 1: Plume centreline for different wind categories (0-5) and their associated stabilities for typical spring days.

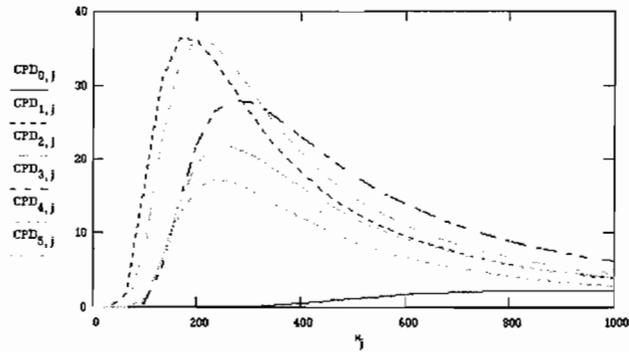


Figure 2: Maximum plume concentrations for different wind categories (0-5) and their associated stabilities for typical spring days. To obtain a pollutant concentration, you must multiply by 1/1.000.000 and its emission.



Figure 3: Average NO_x isoconcentration curves ($\mu\text{g}/\text{Nm}^3$) during spring in day time

10. References

- [1] Briggs, G.A. Diffusion Estimation for Small Emissions. ATDL Contribution File No. 79, Atmospheric Turbulence and Diffusion Laboratory, 1973.
- [2] Britter, R.E. and McQuaid, J. Workbook on the dispersion of dense gases. HSE Contract Research Report No 17/1988. Health and Safety Executive, Sheffield, UK, 129 pp, 1988.
- [3] Cox, R.A. and Carpentier, R.J. Further Development of a Dense Cloud Dispersion Model for Hazard Analysis. In F. Hartwig (ed.), Heavy Gas and Risk Assessment. D. Reidel, Dordrecht FRG, 1980.
- [4] Cramer, H.E. Improved Techniques for Modelling the Dispersion of Tall stack plume. In Proceedings of the Seventh International Technical Meeting on Air Pollution Modelling and its Application, No. 51, NATO/CCMS, pp. 731-780, (NTIS PB 270-799), 1976.
- [5] Eltgroth, M. Complex Hazard Air Release Model (CHARM) Version 6.0 Technical Document, Radian Corporation, Austin, TX 78720, 1990
- [6] Ermark, D.L. SLAB: An Atmospheric Dispersion Model for Dense-Than-Air Releases (Draft, November Version), Lawrence Livermore National Laboratory, Livermore, CA 94550, 1989.
- [7] Ermak, D.L. and Merry, M.H. A Methodology for Evaluating Heavy Gas Dispersion Models. ESL-TR-88-37. AFESC, Tyndall AFB, Florida. 1989.
- [8] Escudier, M.P. Aerodynamics of a Burning Turbulent Gas Jet in a Cross Flow. Combust. Sci. Technol., 4, 193-301. (1972).
- [9] Golder, D. Relations between Stability Parameters in the surface layer. Bound. Layer Meteorol., 3, pp. 46-68, 1972.
- [10] Hanna, S.R.. Applications in air pollution modelling. Ch 7 in Atmospheric Turbulence and Air Pollution Modelling. (F.T.M. Nieuwstadt and H. Van Dop, eds.) D. Reidel, Dordrecht, Holland, pp. 275-310, 1982
- [11] Irwin, J.S. Estimating plume dispersion. A comparison of several sigma schemes. J. Climate Applied Meteorol., 22, pp 92-114, 1983
- [12] Kunkel, B.A. User's guide for the Air Force Toxic Chem. Dispersion Model (AFTOX), AFGL-TR-88-0009. AFGL, Hanscom AFB, MA 01731, 1988.
- [13] Ooms, G., Mahieu, A.P. and Zelis, F. The plume path of vent gases heavier than air. Proc. First Intern. Symp. on Loss Prevention and Safety Promotion in the Process Industries. C.H. Buschman Ed., Elsevier Press, 1974.
- [14] Panofsky, H. and Dutton, J. Atmos. Turbulence. John Wiley & Sons. 1989.
- [15] Pasquill and Dutton. Atmospheric Diffusion, pag. 339, 1983.
- [16] Ricou, F. P. And Spalding, D.B. Measurement of Entrainment by Axialsymmetrical Turbulent Jets. J. Fluid. Mech., 11, 21-32. (1961)
- [17] Servert, J., Crespo, A., Hernández, J. A One-Dimensional Model of a Turbulent Jet Diffusion Flame in an Ambient Atmospheric Flow, Derived from a 3-D Model. Combust. Sci. and Tech., 124, pp 83-114 (1997).
- [18] The American Meteorological Society 1977 Committee on Atmospheric Turbulence and Diffusion
- [19] Tamanini, F. An Integral Model of Turbulent Fire Plumes. Eighteenth Symposium on Combustion, pp. 1081-1090. (1981).