THE NUMERICAL SIMULATION OF THE SPREADING OF A POLLUTANT PLUME IN THE ATMOSPHERE CONSIDERING CHANGE OF PHASE AND TOPOGRAPHY

F. Mayinger; G. Pültz; B. Durst
Chair A for Thermodynamics of the Technical University of Munich, FRG

ABSTRACT

This paper presents a model for the numerical simulation of the spreading of a pollutant plume emanating from a conventionally fired power plant in the atmospheric boundary layer. Besides the basic wind cross flow and chimney exit flow the model considers the influence of topography, thermodynamics and meteorology on the flow field. The model solves the Reynolds-averaged threedimensional partial differential equations resulting from the conservation laws for momentum, energy and mass, using a buoancy modified k,ε turbulence model for the closure of the set of equations. The equations are discretized by means of a finite-volume-method using a deferred correction scheme combining upwind- and central-differences discretization for spatial- and a fully-implicit scheme for time-discretization. The resulting set of algebraic equations is solved incorporating the strongly implicit procedure according to Stone. The model permits reliable predictions of effects caused by a pollutant plume emanating from a power plant on the near environment in advance of the construction of the power plant.

INTRODUCTION

The numerical simulation of the dispersion of airborne pollutants by means of computational fluid dynamics is considered the most important linkage between the information about emissions and their effect upon the near environment. This is especially true for conventionally fired power plants, emitting a number of pollutants, which can not be avoided within the combustion process. Sulfur-dioxid SO_2 and the Nitrogen-oxids NO_x,which in connection with water H_2O yield the so called "Acid Rain" are one example, Carbon-dioxid CO_2, which is believed to be the main cause for the "Green House Effect", another. Besides these more general ecological and climatic problems, there are also regional catastrophies like the accidents of Tschernobyl, Bhopal, Seveso, etc. or the burning oil fields in Kuwait. The only way to inspire confidence within the people is by minimizing the pollution of inhabited regions surrounding such a power plant. Therefore the aim of the work presented is to enhance the capability of predicting the effects of the pollutant plume emanating from a power plant on the near environment in advance of the construction of the power plant.

An Eulerian box model is used, because this model allows to take into account physical phenomena of the pollutant plume in the numerical simulation, which have not - or only in a simple way - been considered so far. The interest is focused on three phenomena, which - besides the basic wind cross flow and chimney exit flow - are looked upon as the most important:

- Topography (3-D-flow over and around obstacles like buildings, houses, etc.)
- Thermodynamics (condensation of water droplets - formation of fog)
- Meteorology (weather classes - thermal stratification of the athmospheric boundary layer)

Therefore the model allows reliable predictions of the influence of a conventionally fired power plant, particularly concerning the plume visibility due to the formation of fog and the shadowing of surrounding houses entailed. Furthermore the peak concentration of pollutants at ground level or on the surface of buildings can be predicted, thereby enabling statements required for approval-procedures.

BASIC EQUATIONS

The partial differential euations gouverning the flow described in the present paper are derived from the conservation laws for mass or mass fraction (concentration), momentum and energy. In order to account for turbulent effects the equations are Reynolds-averaged and formulation for an incompressible Newtonian fluid with constant properties within a Cartesian coordinate system using tensornotation yields:

- momentum-equations (Reynolds-equations):

$$\rho \frac{D\overline{w}_j}{Dt} - \mu \frac{\partial^2 \overline{w}_j}{\partial x_i^2} = \rho a_j - \frac{\partial \overline{p}}{\partial x_j} - \rho \frac{\partial \overline{w_i' w_j'}}{\partial x_i} \qquad (1)$$

- energy-equation (temperature-transport-equation):

$$\rho c_p \frac{D\overline{T}}{Dt} - \lambda \frac{\partial^2 \overline{T}}{\partial x_i^2} = -\rho \frac{\partial \overline{w_i' T'}}{\partial x_i} + \Delta E_{Ph} \tag{2}$$

- continuity-equation:

$$\frac{\partial \overline{w}_i}{\partial x_i} = 0 \tag{3}$$

- concentration-equation:

$$\rho \frac{D\overline{c}}{Dt} - \rho d \frac{\partial^2 \overline{c}}{\partial x_i^2} = -\rho \frac{\partial \overline{w_i' c'}}{\partial x_i} + S_{Ph} \tag{4}$$

neglecting dissipation and temperature variations due to pressure changes in equation (2). The energy-equation includes an additional sink/source term due to the change-of-phase (e.g. condensation → formation of fog), which is calculated as change-of-phase-enthalpy times production rate of droplets

$$\Delta E_{Ph} = r_s \dot{m}_{fl} = r_s \frac{\partial c_{dr}}{\partial t} \tag{5}$$

A corresponding sink/source term appears in the concentration-equation for vapour and together the two invoke an additional coupling of the equations, which reduces the numerical stability.
Within the equations given above turbulence phenomena are considered by the formulation according to Reynolds, splitting independent variables (e.g. velocity, temperature, pressure, etc.) into a time-averaged mean value (signed by an overbar) and a fluctuation (signed by a quote). This entails that the transformed respectively time-averaged partial differential equations (Reynolds-equations) include terms for correlations of fluctuations (e.g. Reynolds-stresses or turbulent fluxes). Besides constitutive laws, a means of modelling these correlations is required in order to complete the set of partial differential equations (PDEs).

Therefore a statistical turbulence model is incorporated in the set of PDEs. In the present work a buoyancy-modified k,ε-model is used (see [4]), which can be described as follows:
The correlations of turbulent fluxes can be written as

$$-\overline{w_i' w_j'} = \nu_t \left(\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} k \tag{6}$$

$$-\overline{w_i' \Phi'} = \frac{\nu_t}{\sigma_t} \frac{\partial \overline{\Phi}}{\partial x_i} \tag{7}$$

with the turbulent viscosity calculated as

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} \tag{8}$$

For the turbulent kinetic energy k and the turbulent dissipation rate ε the following equations are solved:

$$\frac{Dk}{Dt} - \frac{\partial}{\partial x_i} \left[\left(\nu_l + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] = P + G - \varepsilon \tag{9}$$

$$\frac{D\varepsilon}{Dt} - \frac{\partial}{\partial x_i} \left[\left(\nu_l + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] = C_1 \frac{\varepsilon}{k} (P + G)(1 + C_3 R_f) - C_2 \frac{\varepsilon^2}{k} \tag{10}$$

with the production term P as

$$P = \nu_t \frac{\partial \overline{w}_i}{\partial x_j} \left(\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i} \right) \tag{11}$$

the generation term G caused by buoancy as

$$G = -\beta g_i \frac{\nu_t}{\sigma_t} \frac{\partial \overline{T}}{\partial x_i} \tag{12}$$

and the flux-Richardson-number R_f due to the thermal stratification of the atmospheric boundary layer as

$$R_f = \frac{-G}{P+G} \tag{13}$$

The constants used were:

σ_t = turbulent Prandtl-Number

β = thermal coefficient of volume expansion

$C_\mu = 0,09 \quad \sigma_k = 1,0 \quad \sigma_\varepsilon = 1,3$

$C_1 = 1,44 \quad C_2 = 1,92 \quad C_3 = 0,8$

NUMERICAL METHODS

The numerical solution procedure used in the presented model for the set of unsteady, elliptically, partial differential equations can be best described by the following specifications:

- finite-volume-method (conservative, as based upon fluxes)
- fully-implicit approximation of the time-coordinate (no limitation on the size of the time-step)
- combination of central-differencing- and upwind-discretization (known as "Deferred Correction Scheme")
- collocated grid (using interpolation for cell-face velocities described by Peric et al. [3]
- matrix-solver: Strongly-Implicit-Procedure (SIP) according to Stone [8]
- Pressure-velocity coupling: Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) according to Patankar and Spalding [2]
- Evaluations of the density as a function of pressure, temperature and concentration (no Boussinesq-Approximation)

RESULTS

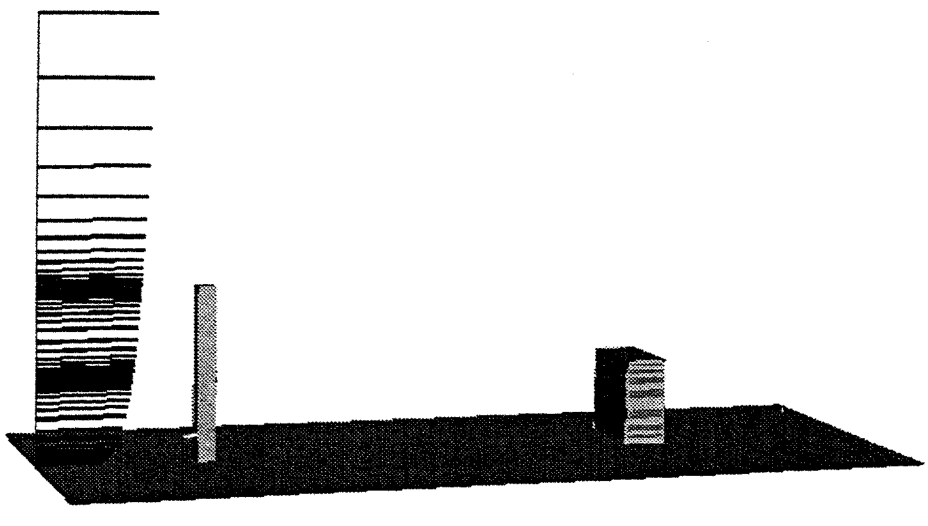

Figure 1: Cross flow wind profile of the atmospheric boundary layer, the emitter and an optional building

In Fig.1 a cross flow wind-profile of the atmospheric boundary layer, a chimney and a building located asymmetrically to the chimney are shown (It is obvious that in this case only 3-D-calculations allow realistic simulations of the flow field). The profile is taken according to the "power-law" as

$$u(z) = u_{ref} \left(\frac{z}{z_{ref}}\right)^{\frac{1}{\alpha}} \tag{14}$$

where the reference-cross-velocity u_{ref} at the reference-height z_{ref} and the exponent α depend strongly on the weather situation. The model presented uses the weather classes according to *Pasquill* (see [1]), which not only provide information about the velocity-profile but also about the thermal stratification of the atmospheric boundary layer, which is important for both the buoyancy and turbulence phenomena.

The influence of the 6 Pasquill classes (A - F) on the spreading of a pollutant plume is shown in Fig. 2.

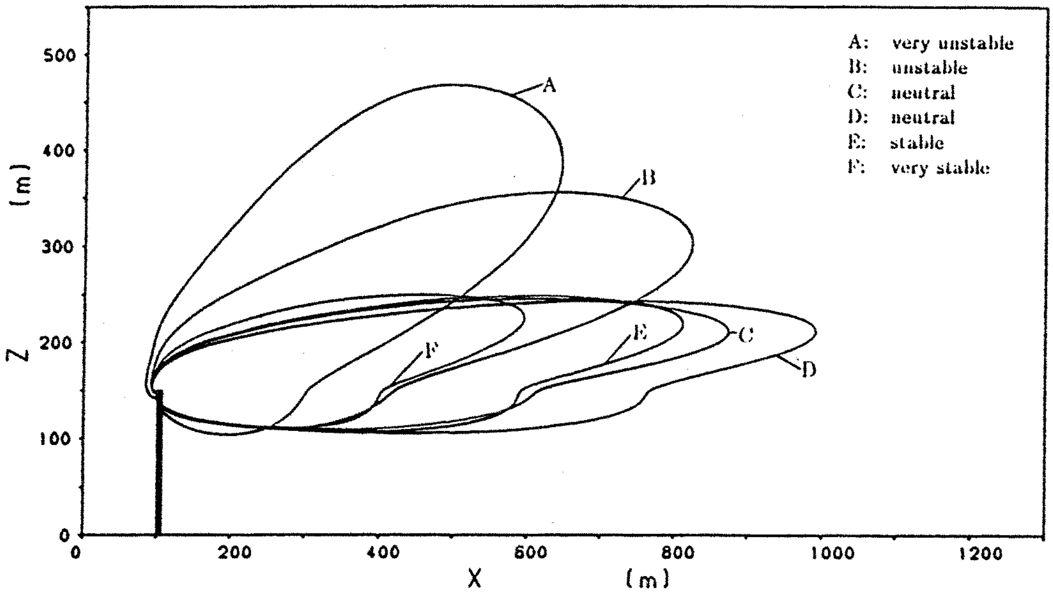

Figure 2: Comparison of the spreading of pollutant plumes for different weather conditions (6 Pasquill classes)

In general the spreading of a plume in the atmospheric boundary layer is dominated by two main transport mechanism: the convective (or advective) transport by the wind field and the so called "turbulent diffusion" due to fluctuations of the flow. Pasquill defines 6 classes for the whole range of weather in such a way, that turbulent diffusion is largest in class A and decreases as the letters advance. In contrast to this the convective transport due to the wind crossflow reaches its maximum value in class D and its minimum values in classes A and F. Using these definitions Pasquill created a scheme, which describes the tendency of the plumes to spread. As plumes of class A spread fastest they are shaped like lumps. Plumes of the opposite class D, which is characterized by the maximum value of the wind cross flow velocity, spread more weakly across the main stream but are transported furthest by the main flow and therefore look more like long and slim tubes. The class with the overall worst spreading is class F as shown in Fig. 2.

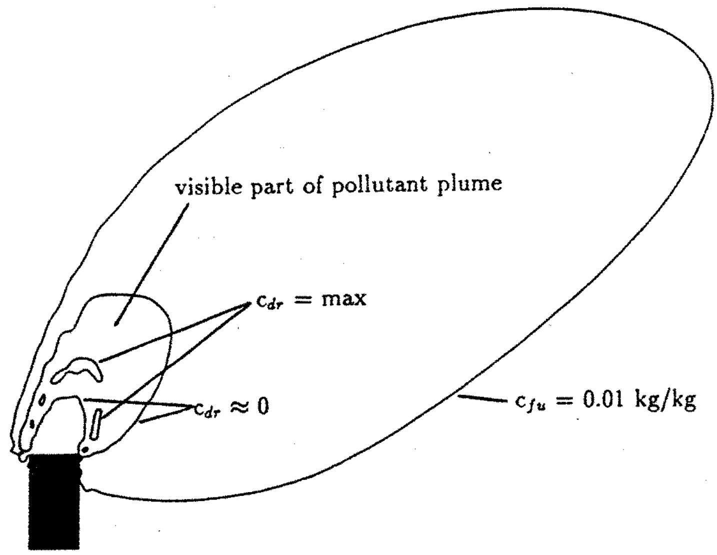

Figure 3: An example for a pollutant plume with change-of-phase phenomena

In Fig. 3 an example of a plume is shown, where the difference between the visible and invisible part of the plume is obvious, with the margin fume-concentration is set to $c_{fu} = 1$ %. The visible part of the plume does not begin immidiately at the chimney exit, because the hot fume has first to be cooled down. Due to this cooling the gas mixture tends to become oversaturated; however the model forces the gas mixture to thermal equilibrium and calculates the condensating water droplets as the difference between the mass fraction of gaseous water actually present and at state of saturation. The visibility of the plume depends - besides dust particles - only on the presence of droplets ($c_{dr} > 0$). Therefore the plume becomes invisible as the droplet-concentration is reduced to zero due to revapourization. As a general statement it is evident, that a plume does not end with its visible part and the extent of the visible part depends of course strongly on the relative humidity of the surrounding air. For example when cold, cloudy and wet weather dominates, the plume is visible much longer than in hot and dry weather as shown in Fig. 3.

The evidence of the reliability of the predictions evaluated by the model presented in this paper is supplied by comparing the predictions with experimental data as shown in Fig. 4.

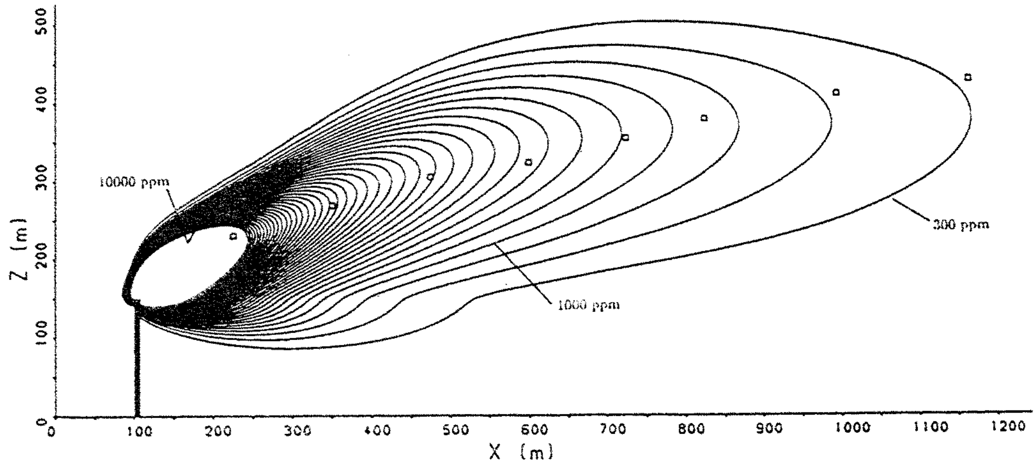

Figure 4: Comparison of experimental measurements with calculated predictions for the power plant of Lakeview

The experimental data used are taken from the work of Slawson and Csanady [5], who measured the extent of a pollutant plumes emanating from the power plant of Lakeview, Canada, in 1965. As they use a visual method for their measurements, they could only determine the trajectories of the plumes. The present model calculates the full spatial distribution of the pollutants and so it does not need to evaluate the trajectories. Therefore in Fig. 4 the trajectory of Csanady's measurements is compared with an isoline of concentration set to a margin value of 0.0003 kg/kg. The agreement between experiments and calculations is satisfying, especially in consideration of the fact that there was no information about the relative turbulent intensity of the crossflow windprofile, which dominates the turbulent diffusion further away from the chimney. The correlations between the results of the experiments and calculations are best in a region surrounding the chimney exit as boundary and starting conditions are determined by measured values in this area and the the spreading is dominated by the turbulence induced by the chimney exit flow.

CONCLUSIONS

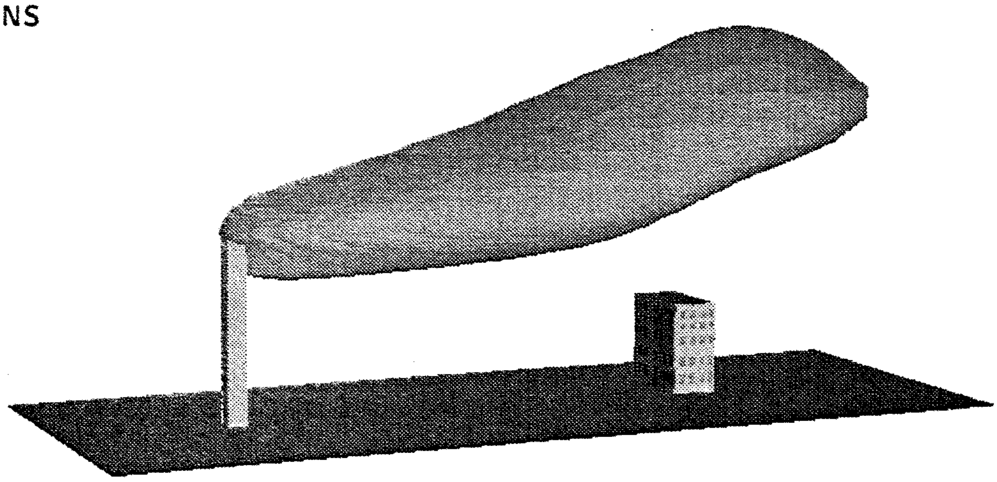

Figure 5: Calculated pollutant plume with margin concentration of 250 ppm

The Use of the model presented in this paper enables the prediction of the time-dependent development and the stationary state of a pollutant plume as shown in Fig. 5. It is thereby possible to estimate influences of the plume on the surroundings of a power plant such as the pollutant concentration on ground level or on the surface of buildings (as shown in Fig. 6) or, as a change-of-phase model is incorporated, the shadowing of houses nearby. However besides such more general qualitative statements the model also permits a detailed quantitative analysis of all values that are fluid dynamically or otherwise of interest. For instance Fig. 6 shows the distribution of a pollutant on the surface of a building located asymmetrically within the wake of the chimney with an offset in the y-direction.

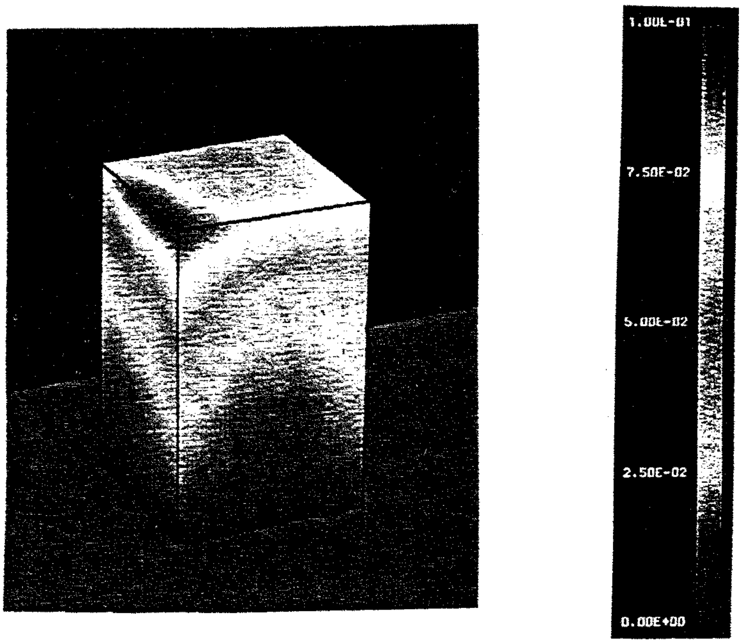

Figure 6: The distribution of a pollutant at the surface of a building located downstream and asymmetric to the emitter

While it is slightly difficult to recognize the value of the concentration, as the original is plotted using colours, the main information of Fig. 6 is that the distribution is predicted asymmetrically according to the location of the building. The maximum value of concentration is found at the top right-hand corner of the building and one can also recognize that the fume-concentration at the vertical corners is higher than on the faces of the building parallel to the main stream. Furthermore the calculations show, that the fume-concentration on rear face of the building is not as high as on the front face, due to the turbulent flow around and over the obstacle.

References

[1] Pasquill, F.: *Atmospheric diffusion: the dispersion of windborne material from industrial and other sources*, D. van Nostrand Company, London, 1962.

[2] Patankar, S.V., Spalding, D.B.: *A Calculation-Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows*, Int. Journal of Heat Mass Transfer, Vol. 15, pp1787-1806, 1972.

[3] Peric, M., Kessler, R., Scheurer, G.: *Comparison of Finite-Volume Numerical Methods with Staggered and Colocated Grids*, Computers & Fluids, Vol. 4, pp389-403.

[4] Rodi, W.: *Turbulent buoyant jets and plumes*, Pergamon Press, University of Karlsruhe, 1982.

[5] Slawson, P.R., Csanady, G.T.: *On the mean path of buoyant, bent-over chimney plumes*, J. Fluid Mechanics, Vol. 28, Part 2, pp311-322, 1967.

[6] Stephan, K., Mayinger, F.: *Thermodynamik, Band 1: Einstoffsysteme*, Springer, Berlin, 1986.

[7] Stephan, K., Mayinger, F.: *Thermodynamik, Band 2: Mehrstoffsysteme und chemische Reaktionen*, Springer, Berlin, 1988.

[8] Stone, H.L.: *Iterative Sollution of Implicit Approximation of Multi-Dimensional Partial Differential Equations*, SIAM Journal of Numerical Analysis, Vol. 5, pp.530-558, 1962.