CHAPTER 4

MATHEMATICAL MODELING AND SIMULATION OF ATMOSPHERIC AIR DISPERSION

4.1 Introduction

Air quality modeling is an essential tool for most air pollution studies. The perfect air pollutant concentration model would allow us to predict the concentration that would result from any specified set of pollutant emissions, for any specified meteorological conditions, at any location, for any time period, with total confidence in our prediction. The best currently available models are far from this ideal. For each type of model, an assessment is made of the model limitation in low wind speed conditions. There is no generally accepted definition of what constitutes a 'low wind speed'. Indeed, the point at which the wind speed may be considered 'low' will depend on the details of the application such as density and concentration, ambient turbulence etc. However, I.G. Lines et al.(1997) implied that wind speeds of less than about 2 m/s can be considered to be low wind speeds. This corresponds to the case where standard meteorological data almost certainly become misleading and the applicability of dispersion models may need to be considered more carefully. All such models are applied to one air pollutant at a time. Most models can be used for several different pollutants, but they must be applied separately to each. No models presented here apply to "air pollution in general." Finally, we give the main practical models for air pollutant dispersion in low wind speed conditions.

4.2 Summary of importance to dispersion modeling

4.2.1 Gaussian models

4.2.1.1 Plume models

Gaussian plume models have been used for a wide variety of purposes for many years, and are described extensively in the literature (e.g. Gifford [1960,1961]). The crosswind concentration in the plume is assumed to have a Gaussian profile, and the standard deviation of the distribution is determined as a function of the downwind distance, the atmospheric stability, the roughness length, etc. These models can be used for continuous or instantaneous releases, and are relatively easy to use.

Gaussian plume models generally predict that the concentration at any fixed downwind location varies in inverse proportion to the mean wind speed. This leads to the models predicting concentrations which tend to infinity as the wind speed approaches zero, and so a limit is usually quoted for the lowest wind speed which may be used in the model. Doury (1980) presented an assessment of the limits to use of 'plume' models for short distances and light wind conditions. He concluded that the results of plume models are less reliable for wind speeds of less than about 2 m/s, below which longitudinal dispersion may become an important factor.

4.2.1.2 Puff models

Puff models are in many ways similar to Gaussian plume models, in that the release is usually considered to have a Gaussian profile. The principal difference is that the release is divided into a sequence of separate 'puffs', each of which is modeled independently, whereas the final concentration at any point is found by superposition of the puffs. The main advantage of these models is that it is relatively easy to model a time-varying release with a wind velocity which varies in direction and magnitude.

Such puff models would appear to be well suited for modeling dispersion in low wind speeds in that they can characterize the inherently variable nature of the wind field, provided appropriate input data are available. Ideally, this would take the form of raw wind data at each time step considered.

4.2.2 Box models

4.2.2.1 Integral plume models

Integral plume models are generally used for the assessment of the near-field dispersion of a continuous, elevated jet release into a crossflow. A set of differential equations for the conservation of momentum, energy, mass etc. is solved simultaneously along the plume, together with various assumptions concerning the rate of air entrainment. The solution of the differential equations gives the plume path and the variation in the centerline plume parameters such as velocity, temperature, concentration etc. The profiles of these parameters across the plume are generally assumed to follow Gaussian forms.

In principle, these models may be applied in low or even zero wind speed conditions. In such calm conditions there would be no momentum transfer to the plume, whose path would then be determined entirely by its own momentum and buoyancy. However, the model can be applied only to the near field. So, although they may not be useful for predicting the distance range of the lower flammable limit, they may be useful for predicting the ranges for accidental releases of most toxic substances.

4.2.2.2 Heavy gas dispersion models

Box models for heavy gas dispersion are similar to integral plume models, except that they generally apply to ground-level releases and incorporate additional spreading of the plume due to the initial density-induced slumping behavior. In the near field, the dispersion is often dominated by this gravity-induced slumping and, as the wind speed has relatively little effect, it is considered that this phase of the modeling would still be appropriate for low wind speeds or calm conditions. However, as the cloud disperses and begins to be affected by the wind, this type of dispersion model assumes that the spread of the cloud is determined by atmospheric turbulence, as for a standard Gaussian plume model.

4.2.3 CFD modeling

Computational Fluid Dynamics or CFD is the analysis of systems involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation. The technique is very powerful and spans a wide range of industrial and non-industrial application areas including one important environmental engineering area: dispersion of pollutants and effluents. The results of CFD modeling would effectively be limited to low wind speed conditions over long periods, unless large eddy simulations are undertaken. However, care would need to be taken that the boundary conditions were adequately specified and that the turbulence model was satisfactory. As the mean wind speed is reduced, so there will be two particular problems in the specification of a turbulence model. The first relates to the fact that, even if the mean wind speed drops to zero, the effective viscosity will approach a constant, the laminar viscosity. The second is that there is almost always residual turbulence in the atmosphere, even at zero mean wind speed. However, CFD modeling is specially valuable when considering dispersion around buildings and complex terrain; some preliminary results from research by the Health and Safety Executive (HSE) are presented by Gilham et.al. (1996) and Havens (1995) has also presented preliminary results of CFD modeling of large-scale dense gas releases in low wind speed conditions.

Havens et al.(1996) analyzed one of the Thorney Island low wind speed trials (Trial 34) using the CFD code MARIAH II. This code used a local turbulence model which simulates Fickian diffusion. The predictions were generally good, although peak concentrations were slightly overestimated.

In this study, the advection diffusion model of interest is developed by Dr. Yukimasa Takemoto et al., Yokkaichi university. This model has been applied to sulphur dioxide dispersion process resulting from stack emission of petrochemical plants in Yokkaichi area. It has been found that simulation results trend to agree well with calculations by the existing one-dimensional plume model (1972) and past measurements (1973). The model's details are described in the next section.

4.3 The advection diffusion model for 3D generalized coordinate system

4.3.1 Governing Equation

A viscous flow is one in which the transport phenomena of friction, thermal conduction and/or mass diffusion are included. The governing three-dimensional equations for an isothermal unsteady, incompressible, viscous flow system are:

a) Equation of continuity

rectangular $$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad (4.1)$$

b) Momentum equation: Navier-Stokes equation

x-component (horizontal)

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)+\frac{\partial P}{\partial x}=\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) \quad (4.2)$$

y-component(vertical upward direction)

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)+\frac{\partial P}{\partial y}=\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)+\rho g_y \quad (4.3)$$

Generally, the term ρg_y may be neglected as in the present work.

z-component (horizontal direction)

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)+\frac{\partial P}{\partial z}=\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right) \quad (4.4)$$

c) Equation of continuity of air pollutant (dispersion equation)

$$\frac{\partial C}{\partial t}+\left(u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}\right)=\frac{\partial}{\partial x}\left(K_H\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_V\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_H\frac{\partial C}{\partial z}\right)+Q \quad (4.5)$$

Here K_H is the horizontal dispersion coefficient, K_V is the vertical dispersion coefficient and Q is amount of pollutant released per volume per unit time.

The above governing equations are written for the rectangular coordinates. To handle non-planar topography or boundary condition, transformation between the physical space using rectangular coordinates with complex finite-difference grid systems to accommodate the non-planar boundary condition and the computational space using terrain-hugging curvilinear/generalized coordinates with rectangular finite-difference grid system is necessary. The type of generalized coordinate system suitable for this transformation is the boundary-fitted coordinate system discussed subsequently in section 4.5. Thus, the independent rectangular coordinates (x, y, z) of the physical planes are to be transformed to a new set of independent variables (ξ, η, ζ) in the computational space where

$$\xi = \xi(x, y, z) \tag{4.6a}$$

$$\eta = \eta(x, y, z) \tag{4.6b}$$

$$\zeta = \zeta(x, y, z) \tag{4.6c}$$

so that the finite-difference grid in the computational space becomes rectangular in shape.

Equations (4.6a) to (4.6c) represent the coordinate transformation involving one or more partial differential equations written in terms of x, y, z and t as the independent variables--- for example; the continuity, momentum and diffusion equations. In these equations, the independent variables x, y and z appear in the partial derivatives and there is the need of replacing the derivatives with respect to x, y, and z in the original partial differential equations with their corresponding derivatives with respect to $\xi, \eta,$ and ζ. This derivative transformation from the original physical space to the computational space given by Equations (4.6a) to (4.6c) makes use of the chain rules of differential calculus as follows:

$$\frac{\partial}{\partial x}=\left(\frac{\partial}{\partial \xi}\right)\left(\frac{\partial \xi}{\partial x}\right)+\left(\frac{\partial}{\partial \eta}\right)\left(\frac{\partial \eta}{\partial x}\right)+\left(\frac{\partial}{\partial \zeta}\right)\left(\frac{\partial \zeta}{\partial x}\right) \quad (4.7)$$

$$\frac{\partial}{\partial y}=\left(\frac{\partial}{\partial \xi}\right)\left(\frac{\partial \xi}{\partial y}\right)+\left(\frac{\partial}{\partial \eta}\right)\left(\frac{\partial \eta}{\partial y}\right)+\left(\frac{\partial}{\partial \zeta}\right)\left(\frac{\partial \zeta}{\partial y}\right) \quad (4.8)$$

$$\frac{\partial}{\partial z}=\left(\frac{\partial}{\partial \xi}\right)\left(\frac{\partial \xi}{\partial z}\right)+\left(\frac{\partial}{\partial \eta}\right)\left(\frac{\partial \eta}{\partial z}\right)+\left(\frac{\partial}{\partial \zeta}\right)\left(\frac{\partial \zeta}{\partial z}\right) \quad (4.9)$$

Equations (4.7), (4.8), and (4.9) allow the derivatives with respect to $x, y,$ and z to be transformed into derivatives with respect to ξ, η and ζ. For example, in the governing equations, such as Equations (4.1), (4.2), (4.3), (4.4), and (4.5), a partial derivative with respect to x can be replaced by Equation (4.7). So can the derivatives with respect to y and z. The coefficients of the derivatives with respect to $\xi, \eta,$ and ζ are called " metrics"; for example, $(\partial\xi / \partial x)$, $(\partial\xi / \partial y)$, $(\partial\eta / \partial x)$ and $(\partial\eta / \partial y)$ are the metric terms which can be obtained from the general transformation given by Equation (4.6a) to (4.6c). However, in many CFD applications, the transformation, Equation (4.6a) to (4.6c), is carried out numerically, and the values of the metric terms are calculated using finite differences. Also, in many applications, the transformation may be more conveniently expressed as the inverse of Equation (4.6a) to (4.6c). The inverse transformation used in this research are written as:

$$x = x(\xi, \eta, \zeta) \quad (4.10)$$

$$y = y(\xi, \eta, \zeta) \quad (4.11)$$

$$z = \dot{z}(\zeta) \quad (4.12)$$

The metrics ($\partial x / \partial \xi$), ($\partial y / \partial \eta$), etc. are defined as the inverse metrics, say, ($\partial \xi / \partial x$), ($\partial \eta / \partial y$), etc. of Equations (4.7), (4.8) and (4.9).

4.3.2 Equations of changes in generalized coordinates

Making use of the chain rule, inverse metrics, and Jacobian determinant, Equations (4.1), (4.2), (4.3), (4.4), and (4.5) are transformed as follows;

Equation of continuity

$$\frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial x}+\frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial x}+\frac{\partial u}{\partial \zeta}\frac{\partial \zeta}{\partial x}+\frac{\partial v}{\partial \xi}\frac{\partial \xi}{\partial y}+\frac{\partial v}{\partial \eta}\frac{\partial \eta}{\partial y}+\frac{\partial v}{\partial \zeta}\frac{\partial \zeta}{\partial y}+\frac{\partial w}{\partial \xi}\frac{\partial \xi}{\partial z}+\frac{\partial w}{\partial \eta}\frac{\partial \eta}{\partial z}+\frac{\partial w}{\partial \zeta}\frac{\partial \zeta}{\partial z}=0 \tag{4.13}$$

The equation of continuity is simplified as follows:

$$J^{-1}\frac{\partial U}{\partial \xi}+J^{-1}\frac{\partial V}{\partial \eta}+J^{-1}\frac{\partial W}{\partial \zeta}=0 \tag{4.14}$$

Here J^{-1} is the inverse of the Jacobian determinant

$$J=\begin{vmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{vmatrix}$$

Three-dimensional Navier-Stokes equation

x-component

$$
\begin{aligned}
&\rho\left[\frac{\partial u}{\partial t}+u\left(\frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial x}+\frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial x}+\frac{\partial u}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)+v\left(\frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial y}+\frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial y}+\frac{\partial u}{\partial \zeta}\frac{\partial \zeta}{\partial y}\right)+\right.\\
&\left.w\left(\frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial z}+\frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial z}+\frac{\partial u}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)\right]=-\frac{\partial P}{\partial \xi}\frac{\partial \xi}{\partial x}-\frac{\partial P}{\partial \eta}\frac{\partial \eta}{\partial x}-\frac{\partial P}{\partial \zeta}\frac{\partial \zeta}{\partial x}+\mu\left[\frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2\right.\\
&+\frac{\partial^2 u}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 u}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 u}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2\\
&\left.+\frac{\partial^2 u}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 u}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 u}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 u}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial x}\right)^2\right]\\
&+\mu\left[\frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2+\frac{\partial^2 u}{\partial \xi\,\partial \eta}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)+\frac{\partial^2 u}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \xi}{\partial y}\right)+\frac{\partial^2 u}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)\right.\\
&+\frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2+\frac{\partial^2 u}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)+\frac{\partial^2 u}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right)+\frac{\partial^2 u}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right)\\
&\left.+\frac{\partial^2 u}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial y}\right)^2\right]+\mu\left[\frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial z}\right)^2+\frac{\partial^2 u}{\partial \xi\,\partial \eta}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 u}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)+\right.\\
&\frac{\partial^2 u}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial z}\right)^2+\frac{\partial^2 u}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 u}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)\\
&\qquad\left.+\frac{\partial^2 u}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)+\frac{\partial^2 u}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial z}\right)^2\right] \qquad (4.15)
\end{aligned}
$$

y-component

$$\rho\left[\frac{\partial v}{\partial t}+u\left(\frac{\partial v}{\partial \xi}\frac{\partial \xi}{\partial x}+\frac{\partial v}{\partial \eta}\frac{\partial \eta}{\partial x}+\frac{\partial v}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)+v\left(\frac{\partial v}{\partial \xi}\frac{\partial \xi}{\partial y}+\frac{\partial v}{\partial \eta}\frac{\partial \eta}{\partial y}+\frac{\partial v}{\partial \zeta}\frac{\partial \zeta}{\partial y}\right)+\right.$$

$$\left.w\left(\frac{\partial v}{\partial \xi}\frac{\partial \xi}{\partial z}+\frac{\partial v}{\partial \eta}\frac{\partial \eta}{\partial z}+\frac{\partial v}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)\right]=-\frac{\partial P}{\partial \xi}\frac{\partial \xi}{\partial y}-\frac{\partial P}{\partial \eta}\frac{\partial \eta}{\partial y}-\frac{\partial P}{\partial \zeta}\frac{\partial \zeta}{\partial y}+\mu\left[\frac{\partial^2 v}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2\right.$$

$$+\frac{\partial^2 v}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 v}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 v}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 v}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2$$

$$\left.+\frac{\partial^2 v}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 v}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 v}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 v}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial x}\right)^2\right]$$

$$\left.+\frac{\partial^2 v}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial y}\right)^2\right]+\mu\left[\frac{\partial^2 v}{\partial \xi^2}\left(\frac{\partial \xi}{\partial z}\right)^2+\frac{\partial^2 v}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)+\frac{\partial^2 v}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)+\right.$$

$$\frac{\partial^2 v}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 v}{\partial \eta^2}\left(\frac{\partial \eta}{\partial z}\right)^2+\frac{\partial^2 v}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 v}{\partial \zeta\,\partial \xi}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)$$

$$\left.+\frac{\partial^2 v}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)+\frac{\partial^2 v}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial z}\right)^2\right]+\rho g_y \tag{4.16}$$

z-component

$$\rho\left[\frac{\partial w}{\partial t}+u\left(\frac{\partial w}{\partial \xi}\frac{\partial \xi}{\partial x}+\frac{\partial w}{\partial \eta}\frac{\partial \eta}{\partial x}+\frac{\partial w}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)+v\left(\frac{\partial w}{\partial \xi}\frac{\partial \xi}{\partial y}+\frac{\partial w}{\partial \eta}\frac{\partial \eta}{\partial y}+\frac{\partial w}{\partial \zeta}\frac{\partial \zeta}{\partial y}\right)+\right.$$

$$\left.w\left(\frac{\partial w}{\partial \xi}\frac{\partial \xi}{\partial z}+\frac{\partial w}{\partial \eta}\frac{\partial \eta}{\partial z}+\frac{\partial w}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right)\right]=-\frac{\partial P}{\partial \xi}\frac{\partial \xi}{\partial z}-\frac{\partial P}{\partial \eta}\frac{\partial \eta}{\partial z}-\frac{\partial P}{\partial \zeta}\frac{\partial \zeta}{\partial z}+\mu\left[\frac{\partial^2 w}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2\right.$$

$$+\frac{\partial^2 w}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 w}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)+\frac{\partial^2 w}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 w}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2$$

$$\left.+\frac{\partial^2 w}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\frac{\partial^2 w}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 w}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\frac{\partial^2 w}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial x}\right)^2\right]$$

$$+\mu\left[\frac{\partial^2 w}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2+\frac{\partial^2 w}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)\left(\frac{\partial \xi}{\partial y}\right)+\frac{\partial^2 w}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \xi}{\partial y}\right)+\frac{\partial^2 w}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)\right.$$

$$+\frac{\partial^2 w}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2+\frac{\partial^2 w}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)+\frac{\partial^2 w}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right)+\frac{\partial^2 w}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right)$$

$$\left.+\frac{\partial^2 w}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial y}\right)^2\right]+\mu\left[\frac{\partial^2 w}{\partial \xi^2}\left(\frac{\partial \xi}{\partial z}\right)^2+\frac{\partial^2 w}{\partial \xi\,\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)+\frac{\partial^2 w}{\partial \xi\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)+\right.$$

$$\frac{\partial^2 w}{\partial \eta\,\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 w}{\partial \eta^2}\left(\frac{\partial \eta}{\partial z}\right)^2+\frac{\partial^2 w}{\partial \eta\,\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial^2 w}{\partial \zeta\,\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)$$

$$\left.+\frac{\partial^2 w}{\partial \zeta\,\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)+\frac{\partial^2 w}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial z}\right)^2\right] \qquad (4.17)$$

Equations (4.15), (4.16) and (4.17) can be rewritten in the following dimensionless advection form.

$$J^{-1}\frac{\partial u}{\partial t}+\frac{\partial}{\partial \xi}J^{-1}(uU+P\frac{\partial \xi}{\partial x})+\frac{\partial}{\partial \eta}J^{-1}(uV+P\frac{\partial \eta}{\partial x})+\frac{\partial}{\partial \zeta}J^{-1}(uW+P\frac{\partial \zeta}{\partial x})$$

$$=\frac{1}{\mathrm{Re}}\left(\frac{\partial}{\partial \xi}J^{-1}\left(M_1\frac{\partial u}{\partial \xi}+M_2\frac{\partial u}{\partial \eta}+M_3\frac{\partial u}{\partial \zeta}\right)+\frac{\partial}{\partial \eta}J^{-1}\left(M_2\frac{\partial u}{\partial \xi}+M_4\frac{\partial u}{\partial \eta}+M_5\frac{\partial u}{\partial \zeta}\right)+\right.$$

$$\left.\frac{\partial}{\partial \zeta}J^{-1}\left(M_3\frac{\partial u}{\partial \xi}+M_5\frac{\partial u}{\partial \eta}+M_6\frac{\partial u}{\partial \zeta}\right)\right) \qquad (4.18)$$

$$J^{-1}\frac{\partial v}{\partial t}+\frac{\partial}{\partial \xi}J^{-1}(vU+P\frac{\partial \xi}{\partial y})+\frac{\partial}{\partial \eta}J^{-1}(vV+P\frac{\partial \eta}{\partial y})+\frac{\partial}{\partial \zeta}J^{-1}(vW+P\frac{\partial \zeta}{\partial y})$$

$$=\frac{1}{\mathrm{Re}}\left(\frac{\partial}{\partial \xi}J^{-1}\left(M_1\frac{\partial v}{\partial \xi}+M_2\frac{\partial v}{\partial \eta}+M_3\frac{\partial v}{\partial \zeta}\right)+\frac{\partial}{\partial \eta}J^{-1}\left(M_2\frac{\partial v}{\partial \xi}+M_4\frac{\partial v}{\partial \eta}+M_5\frac{\partial v}{\partial \zeta}\right)+\right.$$

$$\frac{\partial}{\partial \zeta} J^{-1}\left(M_3 \frac{\partial v}{\partial \xi} + M_5 \frac{\partial v}{\partial \eta} + M_6 \frac{\partial v}{\partial \zeta} \right)\Bigg) + J^{-1} g_y \tag{4.19}$$

$$J^{-1} \frac{\partial w}{\partial t} + \frac{\partial}{\partial \xi} J^{-1}(wU + P \frac{\partial \xi}{\partial z}) + \frac{\partial}{\partial \eta} J^{-1}(wV + P \frac{\partial \eta}{\partial z}) + \frac{\partial}{\partial \zeta} J^{-1}(wW + P \frac{\partial \zeta}{\partial z})$$

$$= \frac{1}{\mathrm{Re}} \left(\frac{\partial}{\partial \xi} J^{-1}\left(M_1 \frac{\partial w}{\partial \xi} + M_2 \frac{\partial w}{\partial \eta} + M_3 \frac{\partial w}{\partial \zeta} \right) + \frac{\partial}{\partial \eta} J^{-1}\left(M_2 \frac{\partial w}{\partial \xi} + M_4 \frac{\partial w}{\partial \eta} + M_5 \frac{\partial w}{\partial \zeta} \right) + \right.$$

$$\left. \frac{\partial}{\partial \zeta} J^{-1}\left(M_3 \frac{\partial w}{\partial \xi} + M_5 \frac{\partial w}{\partial \eta} + M_6 \frac{\partial w}{\partial \zeta} \right) \right) \tag{4.20}$$

Where $\mathrm{Re} = \frac{\rho U_0 h}{\mu}$ (Uchida, T. et al, 1997)

U_0 = free-stream mean velocity

h = the hill height

$$U = \frac{\partial \xi}{\partial x} u + \frac{\partial \xi}{\partial y} v + \frac{\partial \xi}{\partial z} w$$

$$V = \frac{\partial \eta}{\partial x} u + \frac{\partial \eta}{\partial y} v + \frac{\partial \eta}{\partial z} w$$

$$W = \frac{\partial \zeta}{\partial x} u + \frac{\partial \zeta}{\partial y} v + \frac{\partial \zeta}{\partial z} w$$

$$M_1 = \left(\frac{\partial \xi}{\partial x} \right)^2 + \left(\frac{\partial \xi}{\partial y} \right)^2 + \left(\frac{\partial \xi}{\partial z} \right)^2$$

$$M_2 = \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial y} + \frac{\partial \xi}{\partial z} \frac{\partial \eta}{\partial z}$$

$$M_3 = \frac{\partial \xi}{\partial x} \frac{\partial \zeta}{\partial x} + \frac{\partial \xi}{\partial y} \frac{\partial \zeta}{\partial y} + \frac{\partial \xi}{\partial z} \frac{\partial \zeta}{\partial z}$$

$$M_4 = \left(\frac{\partial \eta}{\partial x} \right)^2 + \left(\frac{\partial \eta}{\partial y} \right)^2 + \left(\frac{\partial \eta}{\partial z} \right)^2$$

$$M_5 = \frac{\partial \eta}{\partial x}\frac{\partial \zeta}{\partial x} + \frac{\partial \eta}{\partial y}\frac{\partial \zeta}{\partial y} + \frac{\partial \eta}{\partial z}\frac{\partial \zeta}{\partial z}$$

$$M_6 = \left(\frac{\partial \zeta}{\partial x}\right)^2 + \left(\frac{\partial \zeta}{\partial y}\right)^2 + \left(\frac{\partial \zeta}{\partial z}\right)^2$$

Equation of continuity of air pollutant (dispersion equation):

$$\frac{\partial c}{\partial t} + u\left(\frac{\partial c}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial x} + \frac{\partial c}{\partial \zeta}\frac{\partial \zeta}{\partial x}\right) + v\left(\frac{\partial c}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial y} + \frac{\partial c}{\partial \zeta}\frac{\partial \zeta}{\partial y}\right) + w\left(\frac{\partial c}{\partial \xi}\frac{\partial \xi}{\partial z}\right.$$

$$\left. + \frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial z} + \frac{\partial c}{\partial \zeta}\frac{\partial \zeta}{\partial z}\right) = K_H\left[\frac{\partial}{\partial \xi}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right) + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \xi}{\partial x}\right)\right)\right] +$$

$$K_H\left[\frac{\partial}{\partial \eta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right) + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)^2 + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)\right)\right] +$$

$$K_H\left[\frac{\partial}{\partial \eta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right) + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial x}\right)^2 + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)\right)\right] +$$

$$K_V\left[\frac{\partial}{\partial \xi}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)^2 + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)\left(\frac{\partial \xi}{\partial y}\right) + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \xi}{\partial y}\right)\right)\right] +$$

$$K_V\left[\frac{\partial}{\partial \eta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right) + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)^2 + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)\left(\frac{\partial \eta}{\partial y}\right)\right)\right] +$$

$$K_V\left[\frac{\partial}{\partial \zeta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right) + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial y}\right)\left(\frac{\partial \zeta}{\partial y}\right) + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial y}\right)^2\right]\right. +$$

$$K_H\left[\frac{\partial}{\partial \xi}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)^2 + \frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right) + \frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \xi}{\partial z}\right)\right)\right] +$$

$$K_H\left[\frac{\partial}{\partial \eta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)+\frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)^2+\frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right)\right)\right]+$$

$$K_H\left[\frac{\partial}{\partial \zeta}\left(\frac{\partial c}{\partial \xi}\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)+\frac{\partial c}{\partial \eta}\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right)+\frac{\partial c}{\partial \zeta}\left(\frac{\partial \zeta}{\partial z}\right)^2\right)\right]$$

$$+\,Q \qquad (4.21)$$

To simplify the above equation, it will be rearranged and rewritten as follows:

$$\frac{\partial J^{-1}c}{\partial t}+\frac{\partial J^{-1}cU}{\partial \xi}+\frac{\partial J^{-1}cV}{\partial \eta}+\frac{\partial J^{-1}cW}{\partial \zeta}=K_H\left(\frac{\partial}{\partial \xi}\left(J^{-1}g_1\frac{\partial c}{\partial \xi}+J^{-1}g_2\frac{\partial c}{\partial \eta}+J^{-1}g_3\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+K_H\left(\frac{\partial}{\partial \eta}\left(J^{-1}g_2\frac{\partial c}{\partial \xi}+J^{-1}g_4\frac{\partial c}{\partial \eta}+J^{-1}g_5\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+K_H\left(\frac{\partial}{\partial \zeta}\left(J^{-1}g_3\frac{\partial c}{\partial \xi}+J^{-1}g_5\frac{\partial c}{\partial \eta}+J^{-1}g_6\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+K_V\left(\frac{\partial}{\partial \xi}\left(J^{-1}h_1\frac{\partial c}{\partial \xi}+J^{-1}h_2\frac{\partial c}{\partial \eta}+J^{-1}h_3\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+K_V\left(\frac{\partial}{\partial \eta}\left(J^{-1}h_2\frac{\partial c}{\partial \xi}+J^{-1}h_4\frac{\partial c}{\partial \eta}+J^{-1}h_5\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+K_V\left(\frac{\partial}{\partial \zeta}\left(J^{-1}h_3\frac{\partial c}{\partial \xi}+J^{-1}h_5\frac{\partial c}{\partial \eta}+J^{-1}h_6\frac{\partial c}{\partial \zeta}\right)\right)$$

$$+J^{-1}Q \qquad (4.22)$$

where,

$$g_1=\left(\frac{\partial \xi}{\partial x}\right)^2+\left(\frac{\partial \xi}{\partial z}\right)^2,\quad g_2=\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial x}\right)+\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \eta}{\partial z}\right),$$

$$g_3=\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\left(\frac{\partial \xi}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right),\quad g_4=\left(\frac{\partial \eta}{\partial x}\right)^2+\left(\frac{\partial \eta}{\partial z}\right)^2$$

$$g_5=\left(\frac{\partial \eta}{\partial x}\right)\left(\frac{\partial \zeta}{\partial x}\right)+\left(\frac{\partial \eta}{\partial z}\right)\left(\frac{\partial \zeta}{\partial z}\right),\quad g_6=\left(\frac{\partial \zeta}{\partial x}\right)^2+\left(\frac{\partial \zeta}{\partial z}\right)^2,$$

$$h_1 = \left(\frac{\partial \xi}{\partial y}\right)^2 \qquad , h_2 = \frac{\partial \xi}{\partial y}\frac{\partial \eta}{\partial y} \qquad , h_3 = \frac{\partial \xi}{\partial y}\frac{\partial \zeta}{\partial y}$$

$$h_4 = \left(\frac{\partial \eta}{\partial y}\right)^2 \qquad , h_5 = \frac{\partial \eta}{\partial y}\frac{\partial \zeta}{\partial y} \qquad , h_6 = \left(\frac{\partial \zeta}{\partial y}\right)^2$$

$$J = \begin{vmatrix} \dfrac{\partial \xi}{\partial x} & \dfrac{\partial \xi}{\partial y} & \dfrac{\partial \xi}{\partial z} \\ \dfrac{\partial \eta}{\partial x} & \dfrac{\partial \eta}{\partial y} & \dfrac{\partial \eta}{\partial z} \\ \dfrac{\partial \zeta}{\partial x} & \dfrac{\partial \zeta}{\partial y} & \dfrac{\partial \zeta}{\partial z} \end{vmatrix}$$

In next steps, equations of the changes in generalized coordinate system will be discretised by using 3D QUICK scheme (Takemoto,Y. et al.,1986). After applying 3D QUICK scheme to the nonlinear terms with the help of the finite difference approximation equation (within each control volume), Adams-Bashforth algorithm is used to execute numerical time integration (Takemoto,Y. et al.,1996). Further discussion of these schemes is given in the next section.

4.4 The discretisation scheme and numerical method

In this section, the upwind finite-difference scheme is introduced in order to reduce truncation errors and enhance numerical stability. The use of upwind quantities ensures that the scheme are very stable and obey the transportiveness requirement but the resulting first-order accuracy makes them prone to errors caused by numerical dissipation (artificial viscosity) and numerical dispersion (artificial diffusion) (J.D. Anderson.,1995). Such errors can be minimized by employing high-order discretisation. Higher-order schemes involve more neighboring points and reduce the discretisation errors by bringing in more approximation terms. The QUICK scheme is the one of the widely used upwind schemes with high order of accuracy.

4.4.1 Quadratic upwind differencing scheme: the QUICK scheme

In the present study, the solution procedure uses spatially third-order accurate upwind difference technique based on the QUICK algorithm that has been extended to generalized coordinates. The QUICK method was developed by Leonard (1983&1984).

For example, Navier-Stokes equation is to be integrated over the control-volume computing cell on a uniform regular grid shown in Figure 4.1.

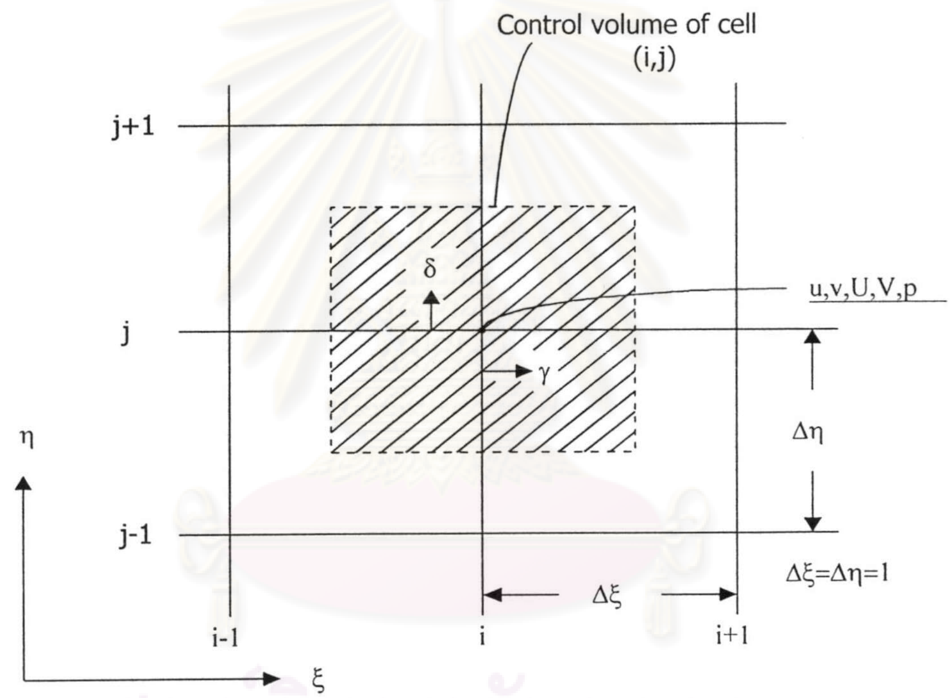


Figure 4.1 Schematics of a transformed computational grid.

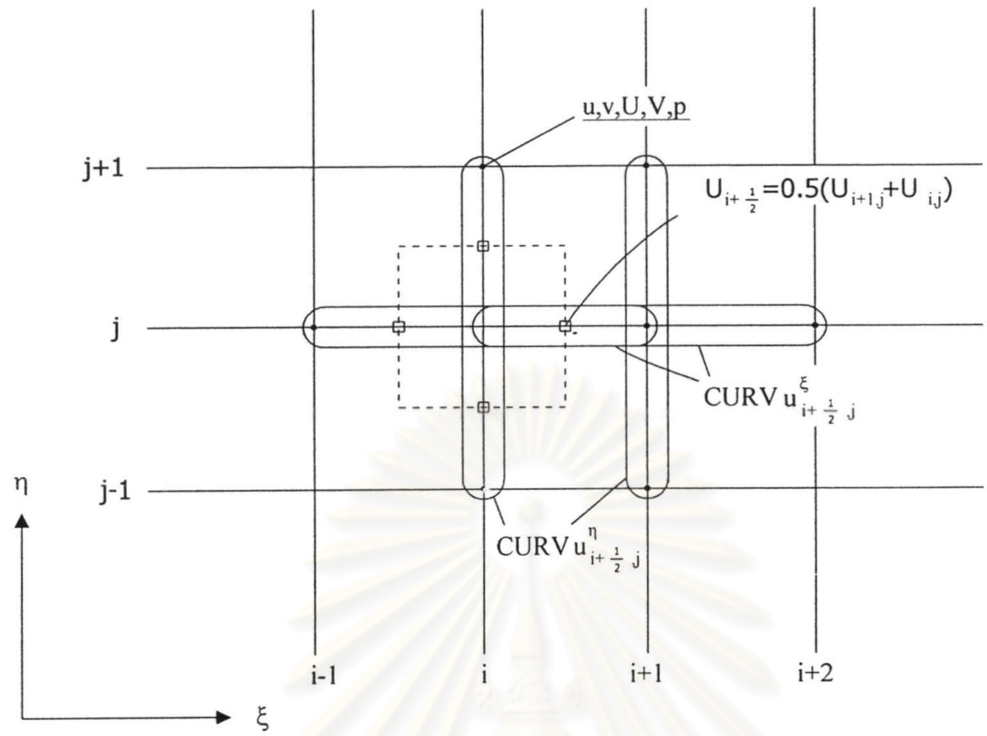


Figure 4.2 Parabolic interpolation by curvature terms

This involves the use of local coordinates (γ,δ,λ) at nodes (i,j,k) of the finite difference grid where $\gamma=\xi-\xi_i$, $\delta=\eta-\eta_j$ and $\lambda=\zeta-\zeta_k$. In equation (4.18), consider one of the nonlinear terms in the x-momentum equation, $(J^{-1}uU)$, to get the following:

$$\int_{\frac{-\Delta\xi}{2}}^{\frac{\Delta\xi}{2}}\int_{\frac{-\Delta\eta}{2}}^{\frac{\Delta\eta}{2}}\int_{\frac{-\Delta\zeta}{2}}^{\frac{\Delta\zeta}{2}}\frac{\partial}{\partial\xi}\left(J^{-1}uU\right)d\lambda\, d\delta\, d\gamma=\int_{\frac{-\Delta\eta}{2}}^{\frac{\Delta\eta}{2}}\int_{\frac{-\Delta\zeta}{2}}^{\frac{\Delta\zeta}{2}}\left[\left(J^{-1}uU\right)_{i+\frac{1}{2},j,k}-\left(J^{-1}uU\right)_{i-\frac{1}{2},j,k}\right]d\lambda\, d\delta \tag{4.23}$$

Here, apply third-order-accuracy upstream control volume scheme 3D QUICK method for $(J^{-1}uU)_{i+\frac{1}{2},j,k}$ to obtain

$$\left(J^{-1}uU\right)_{i+\frac{1}{2},j,k} = \left(J^{-1}U\right)_{i+\frac{1}{2},j,k}\left[\frac{1}{2}(u_{i+1,j,k} + u_{i,j,k}) - \frac{\Delta\xi^2}{8} CURV\, u^{\xi}{}_{i+\frac{1}{2},j,k} + \frac{\Delta\eta^2}{24} CURV\, u^{\eta}{}_{i+\frac{1}{2},j,k} + \frac{\Delta\zeta^2}{24} CURV\, u^{\zeta}{}_{i+\frac{1}{2},j,k}\right] \quad (4.24)$$

Here the curvature terms using parabolic interpolation (CURV) and depending on the direction of the contravariant velocity U in Fig 4.2 would be

$$CURV\, u^{\xi}{}_{i+\frac{1}{2},j,k} = \begin{cases} \left(\dfrac{u_{i+1,j,k} - 2u_{i,j,k} + u_{i-1,j,k}}{\Delta\xi^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} > 0 \\ \left(\dfrac{u_{i+2,j,k} - 2u_{i+1,j,k} + u_{i,j,k}}{\Delta\xi^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} < 0 \end{cases} \quad (4.25)$$

$$CURV\, u^{\eta}{}_{i+\frac{1}{2},j,k} = \begin{cases} \left(\dfrac{u_{i,j+1,k} - 2u_{i,j,k} + u_{i,j-1,k}}{\Delta\eta^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} > 0 \\ \left(\dfrac{u_{i,j+2,k} - 2u_{i,j+1,k} + u_{i,j,k}}{\Delta\eta^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} < 0 \end{cases} \quad (4.26)$$

$$CURV\, u^{\zeta}{}_{i+\frac{1}{2},j,k} = \begin{cases} \left(\dfrac{u_{i,j,k+1} - 2u_{i,j,k} + u_{i,j,k-1}}{\Delta\zeta^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} > 0 \\ \left(\dfrac{u_{i,j,k+2} - 2u_{i,j,k+1} + u_{i,j,k}}{\Delta\zeta^2}\right) & , j^{-1}U_{i+\frac{1}{2},j,k} < 0 \end{cases} \quad (4.27)$$

A regular grid matching $u, v, w, U, V W,$ and P is used. Thus, in terms of two dimensions, $CURV\, u^{\xi}$ for the control volume plane $\left(i+\frac{1}{2}, j, k\right)$

becomes a three-point interpolation in accordance with the upwind direction $u_{i+\frac{1}{2},j,k}$ such as given in Figure 4.2. The upstream side may be selected according to the wind direction for $CURV\, u^{\eta}$ and $CURV\, u^{\zeta}$ of intersection directions.

4.4.2 Numerical time integration method (fractional step method)

First, divide the integration process into two steps. In step 1, take into consideration the convection terms and half of the viscous (dissipation) term and in this case apply the Adams-Bashfort scheme. The Adams-Bashfort scheme, whose principle is based on Taylor series expansion, is used to integrate the variables with respect to time.

$$y_{t+1} = y_t + \Delta t\left(\frac{3}{2}f_t - \frac{1}{2}f_{t-1}\right) + O\left(h^3\right) \tag{4.28}$$

where, $O(h^3)$ is the third-order error term.

f_t, f_{t-1} are the first-order derivative of y with respect to to t at time t and t-1, respectively.

In step 2, the remaining viscosity and pressure terms are solved by an implicit method.

4.5 Boundary-fitting coordinates (Y. Takemoto et al., 1996)

The concept of the boundary-fitting coordinate system is based on the solutions of suitable elliptic partial differential equations to generate boundary-fitting curvilinear coordinates. The solution of the elliptic partial differential equations for the case of a ground protrusion generally allows smooth generation of the curvilinear coordinates.

A two-dimensional example using an O-Grid to explain the principle is shown in Figure 4.3. Transformation of the curves in the physical plane (x, y) to straight in the computational plane. (ξ,η) is provided by the following equations.

$$\xi = \xi\ (x,y) \tag{4.29}$$

$$\eta = \eta\ (x,y) \tag{4.30}$$

Here y and η represent the vertical coordinates. In Figure 4.3, to transform the points on the physical plane, the following Poisson equation, an elliptic partial differential equation in terms of ξ and η, is solved to generate the curvilinear coordinates (ξ,η)

$$\frac{\partial^2\xi}{\partial x^2}+\frac{\partial^2\xi}{\partial y^2}=R(\xi,\eta) \tag{4.31}$$

$$\frac{\partial^2\eta}{\partial x^2}+\frac{\partial^2\eta}{\partial y^2}=S(\xi,\eta) \tag{4.32}$$

Using suitable inhomogeneous functions $R(\xi,\eta)$ and $S(\xi,\eta)$, grid points can be transformed to cluster near a specific point or a specific coordinate line. In the reverse transformation, the independent variables and the dependent variables are interchanged as in the following equations:

$$\alpha\frac{\partial^2 x}{\partial\xi^2}-2\beta\frac{\partial^2 x}{\partial\xi\partial\eta}+\gamma\frac{\partial^2 x}{\partial\eta^2}=-J^2\left(R\frac{\partial x}{\partial\xi}+S\frac{\partial x}{\partial\eta}\right) \tag{4.33}$$

$$\alpha\frac{\partial^2 y}{\partial\xi^2}-2\beta\frac{\partial^2 y}{\partial\xi\partial\eta}+\gamma\frac{\partial^2 y}{\partial\eta^2}=-J^2\left(R\frac{\partial y}{\partial\xi}+S\frac{\partial y}{\partial\eta}\right) \tag{4.34}$$

The coefficients of the above is:

$$\alpha = \frac{\partial x}{\partial \eta}\frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \eta}\frac{\partial y}{\partial \eta}$$

$$\beta = \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta}$$

$$\beta = \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \xi} + \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \xi}$$

with $x = x(\xi,\eta)$, $y = y(\xi,\eta)$

Here the Jacobian J of the coordinate transformation is:

$$J = \left|\frac{\partial(x,y)}{\partial(\xi,\eta)}\right|$$

$$= \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}$$

Concerning the functions R and S in the present CFD model, the grid can be drawn toward the bottom in the y direction, so that function R can be assigned the value zero, and the following standard normal distribution function is used:

$$R(\xi,\eta) = 0.0 \qquad (4.35)$$

$$S(\xi,\eta) = -0.5 * \sum (\exp(-\frac{a_j^2}{2})) \qquad (4.36)$$

where a_j is standard normal variate at height j (Y. Takemoto et al., 1996)

For simplicity the transformation of the non-planar physical surface is carried out by means of the above boundary fitting curves with the z component being fixed for each curve in order to simplify the transformation. As a result, the curved physical plane $(x,y,z)_z$ at a fixed z is transformed to a corresponding rectangular computational plane $(\xi,\eta,\zeta)_\zeta$ at a constant corresponding ζ. The above elliptic partial differential equation is solved again when z is moved to new neighboring z and the relation between the physical plane $(x,y,z)_z$ and the computational plane $(\xi,\eta,\zeta)_\zeta$ is thus obtained at the new z.

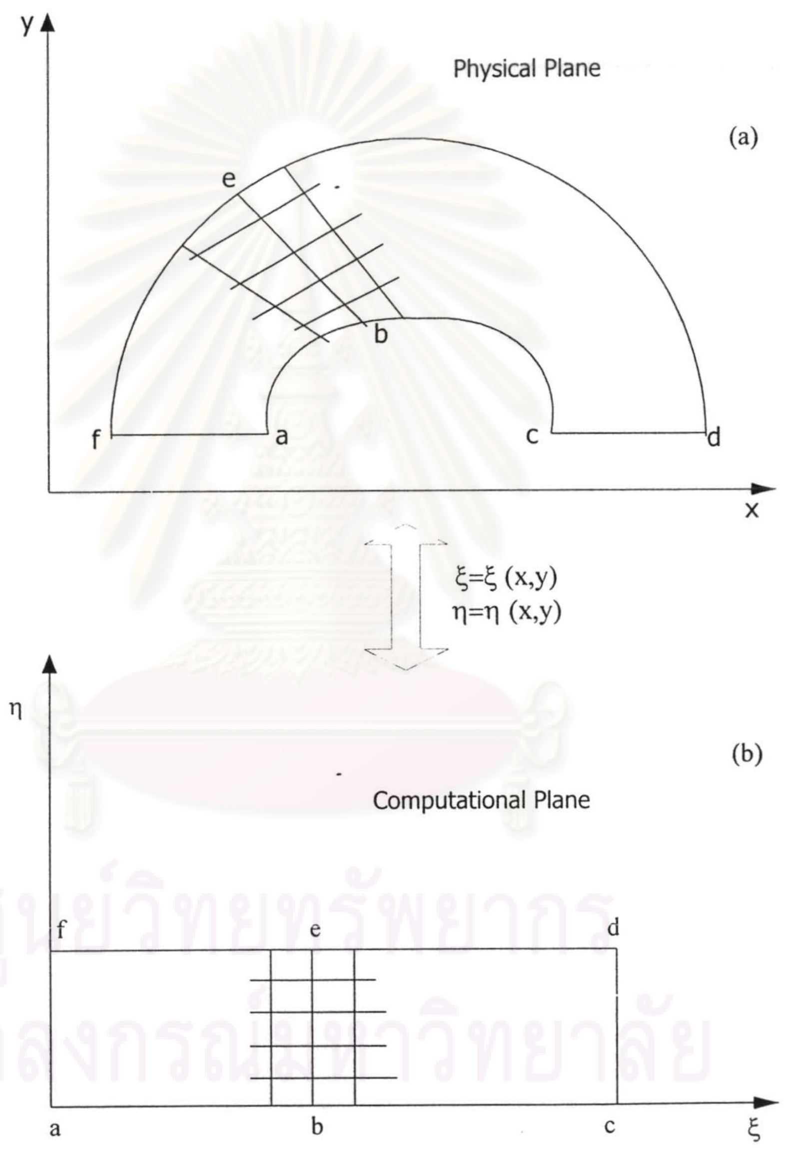


Figure 4.3 (a) Physical plane; (b) Computational plane.

4.6 Assumption used in the present model

For simplicity, the present model is based on the following assumptions:

1. The investigated system consists of chemically non-reactive air pollutants.
2. The air flow is assumed to be isothermal, incompressible and viscous.
3. The wind direction and wind speed are kept constant during the entire period of simulation.

Since the equation of motion does not cover the case of high Re or the turbulence effect, the velocity and pressure field is not accurate if significant turbulence exists. However, the values of the horizontal and vertical dispersion coefficients in the equation of dispersion are obtained by accounting for the combination of diffusion effect and turbulence effect. In other words, the absence of turbulence terms in the equation of motion is compensated to some extent in the equation of dispersion by the high values of horizontal and vertical dispersion coefficients.

4.7 Algorithm of the present model

Simulation is a powerful tool for solving a wide variety of problems. To simulate is to imitate the behavior of a system or phenomenon under study. The basic idea behind dynamic simulation is simple, namely, to model the given system by means of the mathematical equations, and then determine its time-dependent behavior. The simplicity of the approach, when combined with the computational power of a high-speed digital computer, makes simulation a powerful tool. Normally, simulation is used when either an exact analytic expression for the behavior of the system under investigation is not available, or the analytical solution is to time-consuming or costly to obtain.

In this section the simulation algorithm for determining the wind velocity profile and spatial concentration distribution of the dispersed air pollutant are presented and their simplified flow charts are illustrated in Figures 4.4 through 4.10. The simulation is carried out according to the following steps:

1. Survey the topography of the area of interest.

2.To enhance computational precision, create a three-dimensional grid over the entire physical space corresponding to the rectangular gird system on the computational space using a coordinate system adapted to the topography (generalized curvilinear coordinates (ξ,η,ζ)) by solving equations (4.33) and (4.34) for each constant value of ζ . The results are used to create a "Grid Data" file.

3.To calculate the three-dimensional wind velocity field over the physical space of interest from the equation of motion, a high-precision finite-difference scheme (equation (4.28)) and the above generalized coordinate system are employed in the solution of the Navier-Stokes equation, (4.15)-(4.17), as follows:

3.1 Transform the equations of continuity and Navier-Stokes in the physical space (x, y, z) into equations in three-dimensional computational space of generalized coordinates (ξ,η,ζ).

3.2 Input data, including number of grid points in the x, y and z physical space, grid size ($\Delta x,\Delta y,\Delta z$), integration time step size (Δt), Reynolds number, exponent of the power law (pow), measured wind direction (WD), measured wind speed (u_o), and measuring height of the wind speed (y_o) etc.

3.3 Read grid positions (x, y, z) vs. (ξ,η,ζ) and corresponding values of the relevant metrics from "Grid Data" file.

3.4 Initialize all values of the upper atmospheric wind velocity u (velocity in x direction) and w (velocity in z direction) at various heights except y = 0 using the power law and u_o(the measured velocity at hight y_o). It is assumed that the vertical wind speed v

is essentially zero. as for y = 0 (ground surface), u, v and w are assigned to be zero.

3.5 Set the following boundary conditions in the computational space:

-On ground surface (j=1), all u, v, and w in both spaces are zero.

-At j = jmax, u and w in the physical space are estimated by the power law and v is assigned to be zero.

-At i =1 and imax, u and w in the physical space are estimated by the power law and v is assigned to be zero.

-At k =1 and kmax, u and w in the physical space are estimated by the power law and v is assigned to be zero.

3.6 Calculate u, v and w at various x, y, and z in the physical space by solving the transformed Navier-Stokes equation in the computational space using 3D-QUICK and Adams-Bashforth schemes, then mapping the values back onto the physical plane.

3.7 Check if both sums of errors between updated u_n and old u and between the updated v_n and old v are less than epsilon. If it is, assign the latest cycle to be the i^{th} icycle ($cycle_{max}$).

3.8 Check if the cycle value is greater than or equal to the specified value of icycle. If it is, go to the next step. If it is not, let cycle = cycle+1, and return to step 3.6.

3.9 Write the output data, i.e. u, v and w in the physical space onto the designated file.

4. Taking the wind field obtained from the above steps to be the inputs of the dispersion equation.

5.To predict the concentration distribution of the air pollutant, the concentration field calculation is carried out by overlapping with the same generalized coordinates used for the flow field calculation in the computational space. The calculation steps are as follows:

5.1 Transform the dispersion equation in the rectangular coordinates (x, y, z) of the physical space into the corresponding equation in the three-dimensional generalized coordinates (ξ,η,ζ) of the computational space.

5.2 Input data, i.e. number of grid points in the x, y and z space, grid size ($\Delta x,\Delta y,\Delta z$), step size ($\Delta t$), K_H, K_V.

5.3 Read grid positions in the physical space from "Grid Data" file and the wind field data from the output file of step 3.9.

5.4 Set boundary conditions in the computational space as described in "Bound Subroutine" flowchart in Figure 4.10.

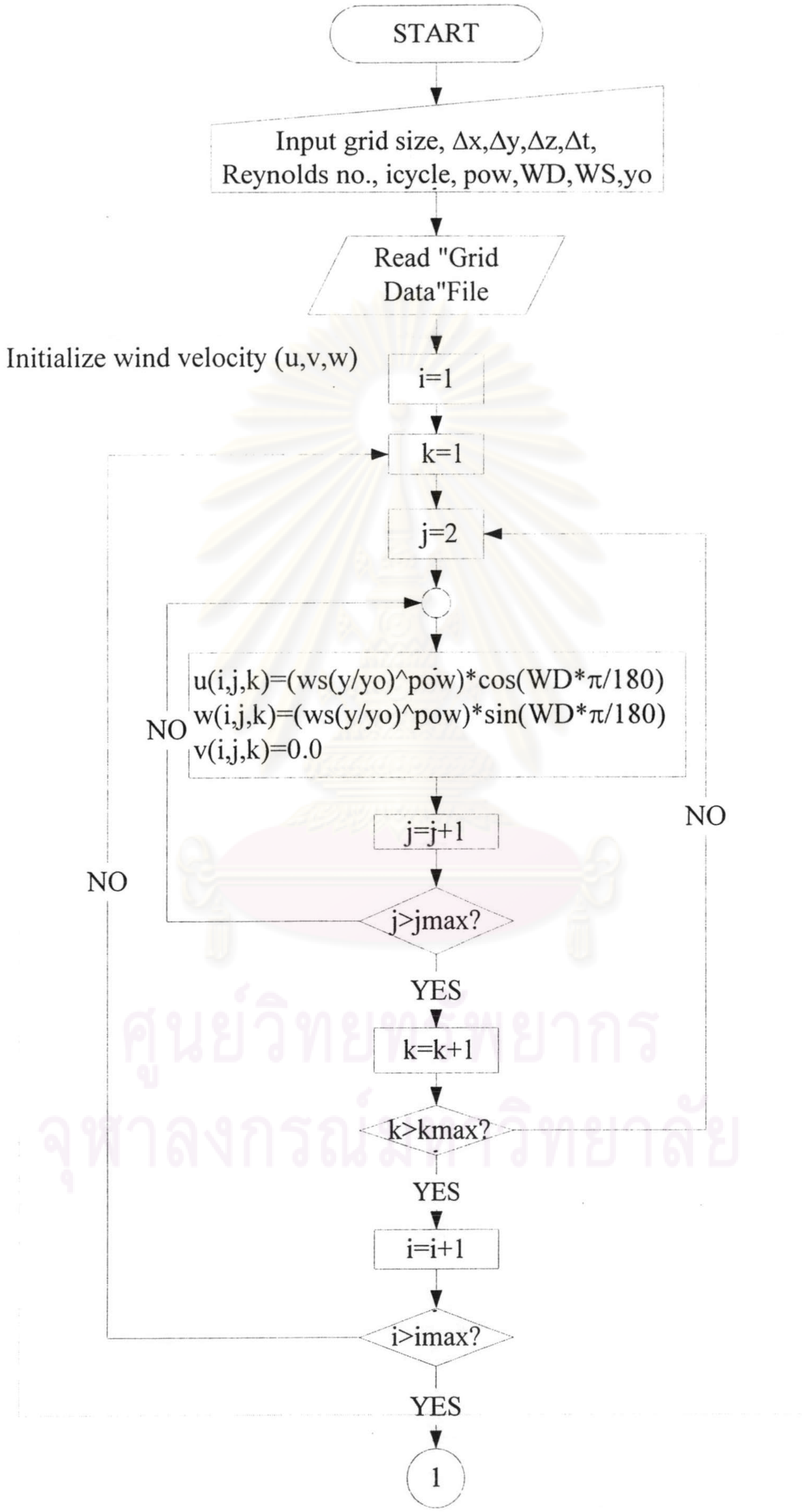
5.5 Calculate the concentration distribution the computational space using the transformed dispersion equation combined with 3D-QUICK and Adams-Bashforth schemes.

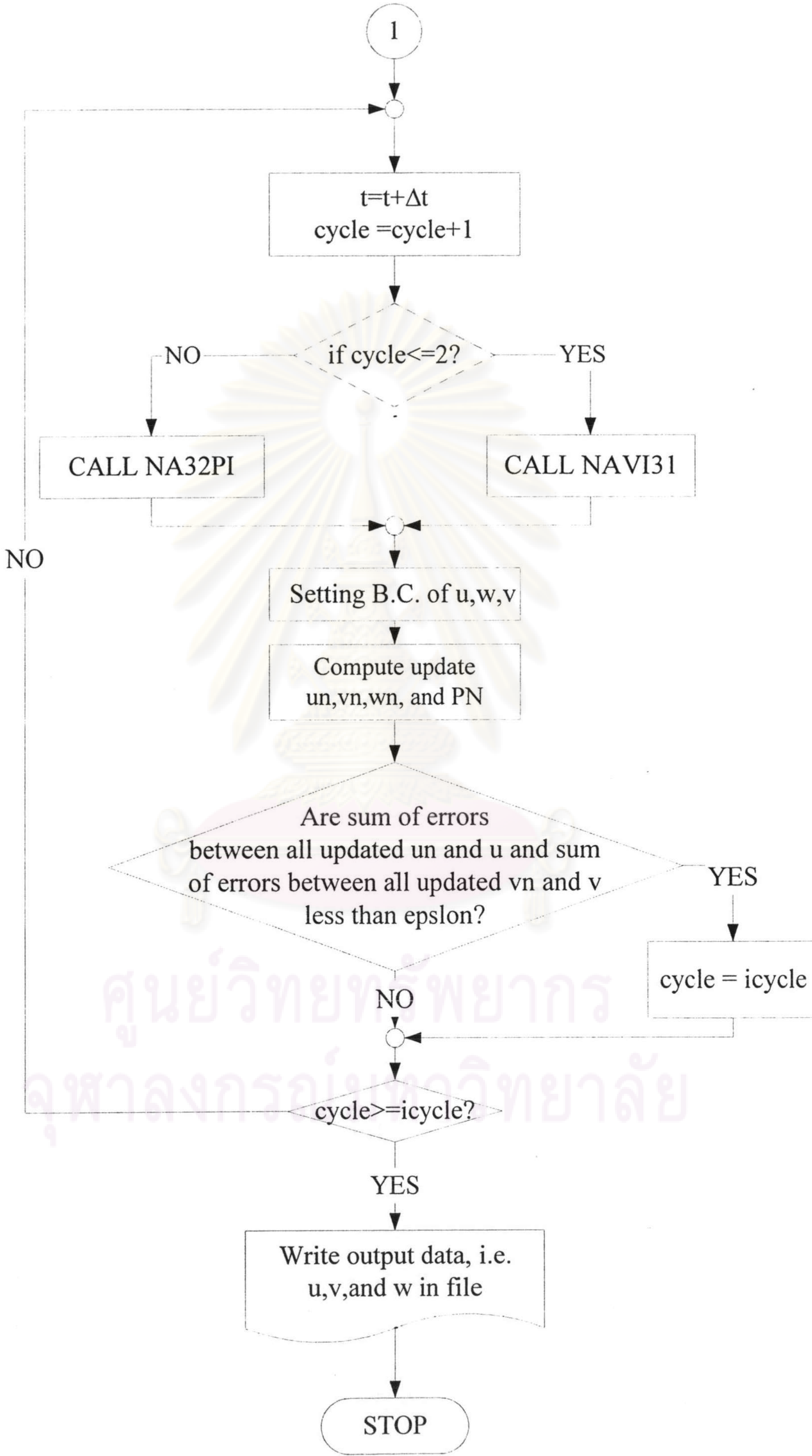
5.6 Check if it is the time to display the results. If it is, go to the next step. If not, skip to step 5.8.

5.7 Transform the concentration distribution in the computational space back onto the physical space. Write the output the data onto designated file.

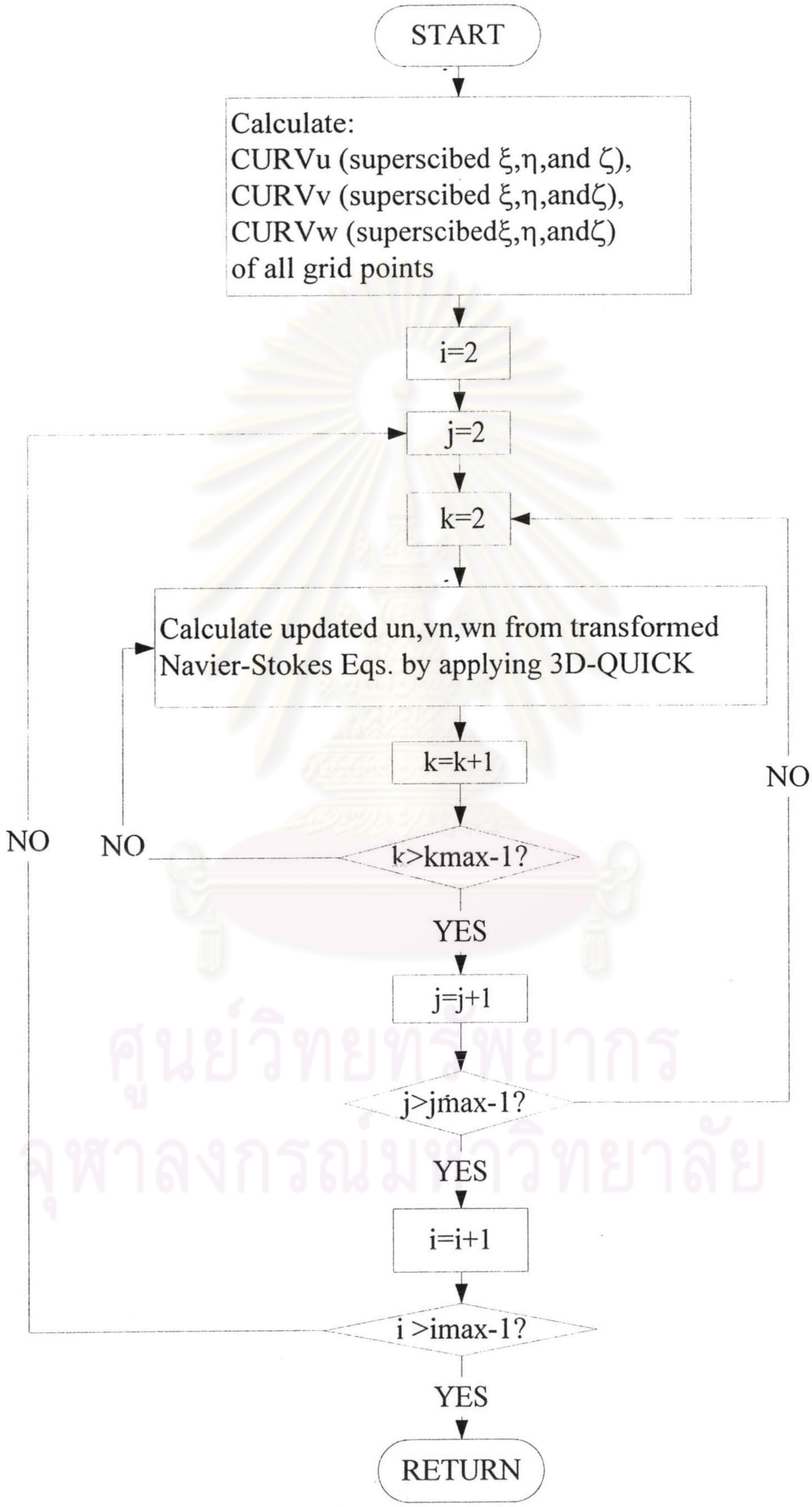
5.8 If the final time has been reached, the simulation is ended. Otherwise, return to step 5.5.

Main Program for Wind Field Calculation

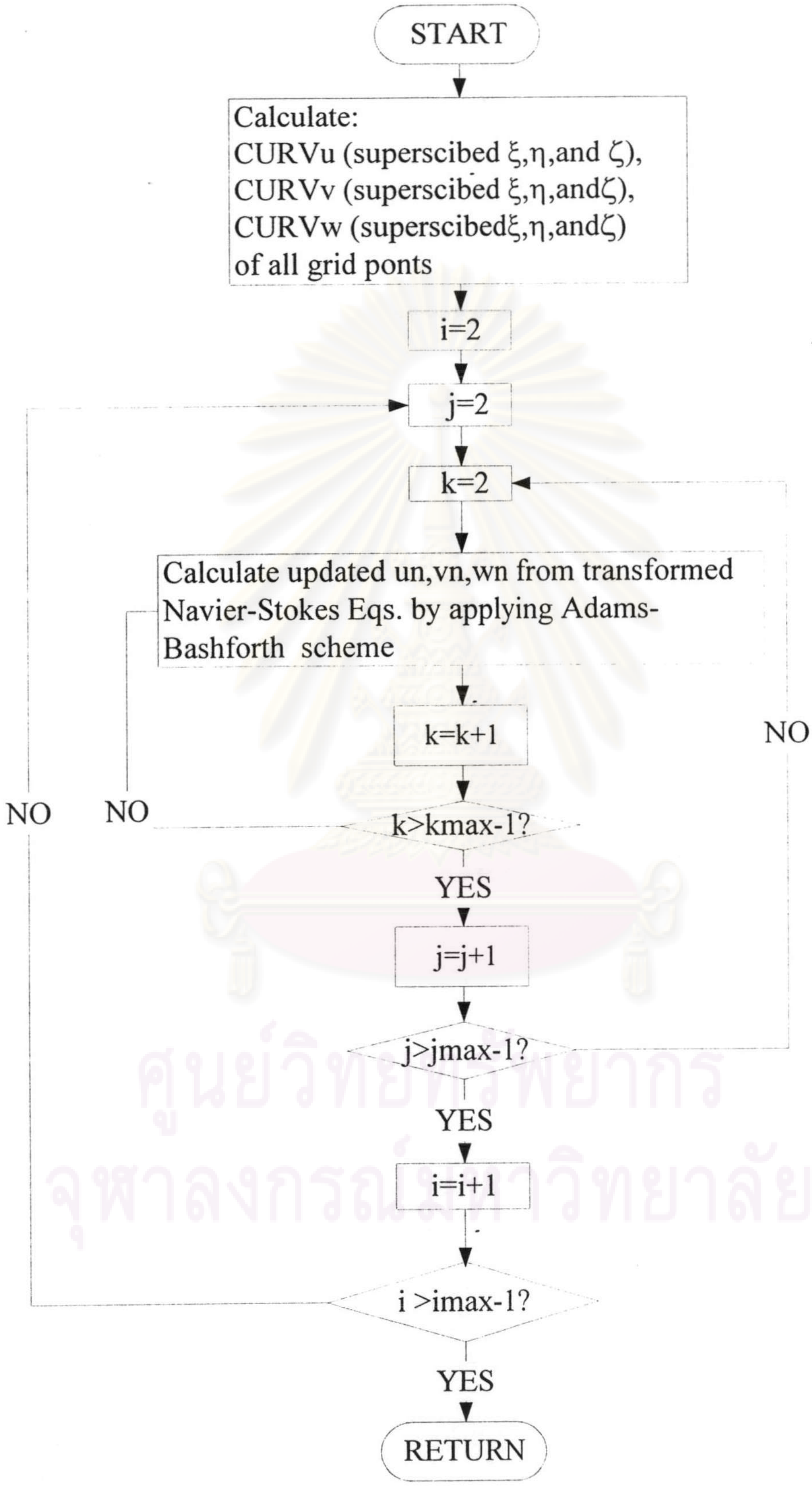



1
t=t+Δt
cycle =cycle+1
if cycle<=2?
NO
YES
CALL NA32PI
CALL NAVI31
NO
Setting B.C. of u,w,v
Compute update
un,vn,wn, and PN
Are sum of errors
between all updated un and u and sum
of errors between all updated vn and v
less than epslon?
YES
cycle = icycle
NO
cycle>=icycle?
YES
Write output data, i.e.
u,v,and w in file
STOP

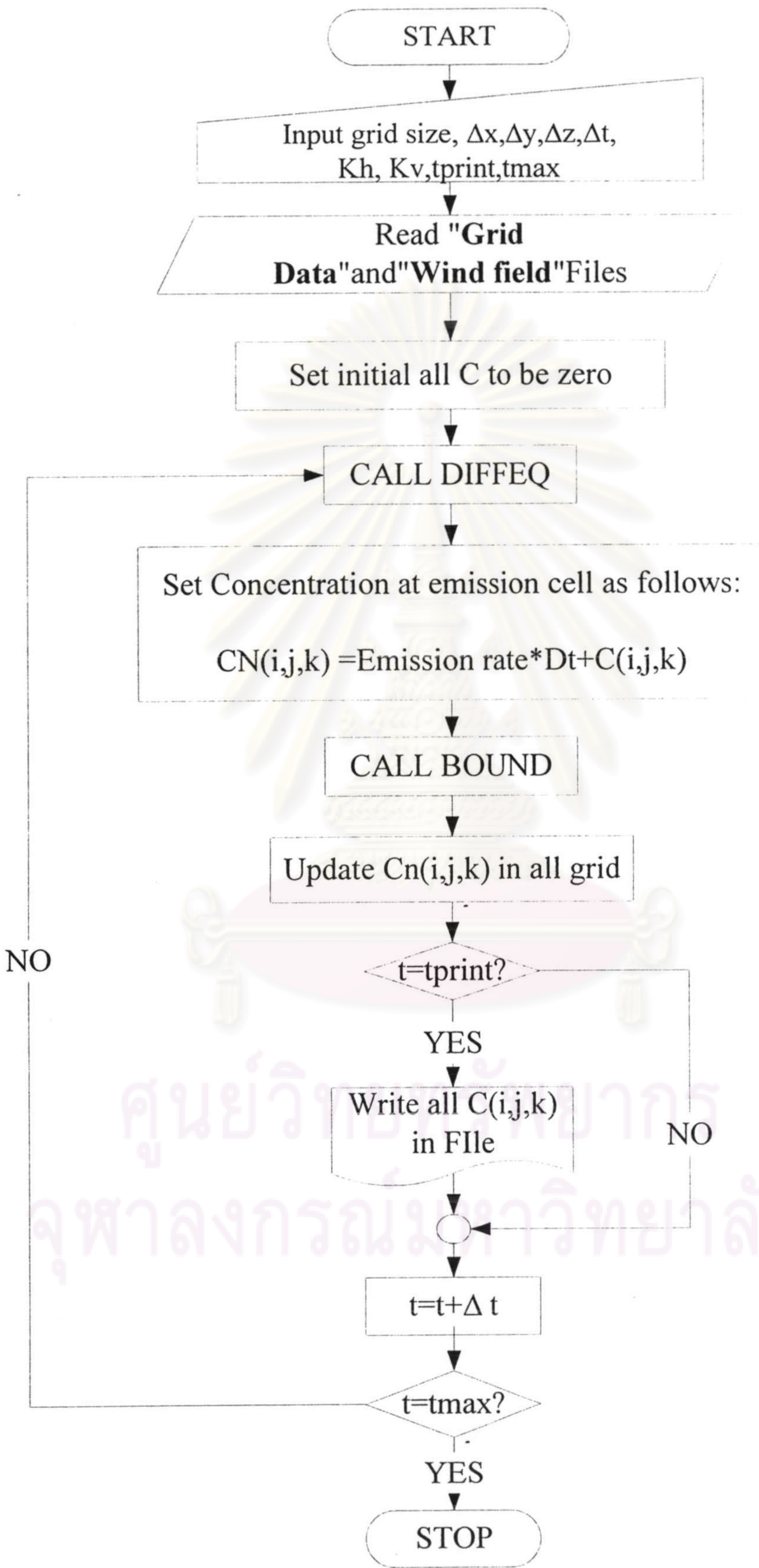
NAVI31 SUBROUTINE



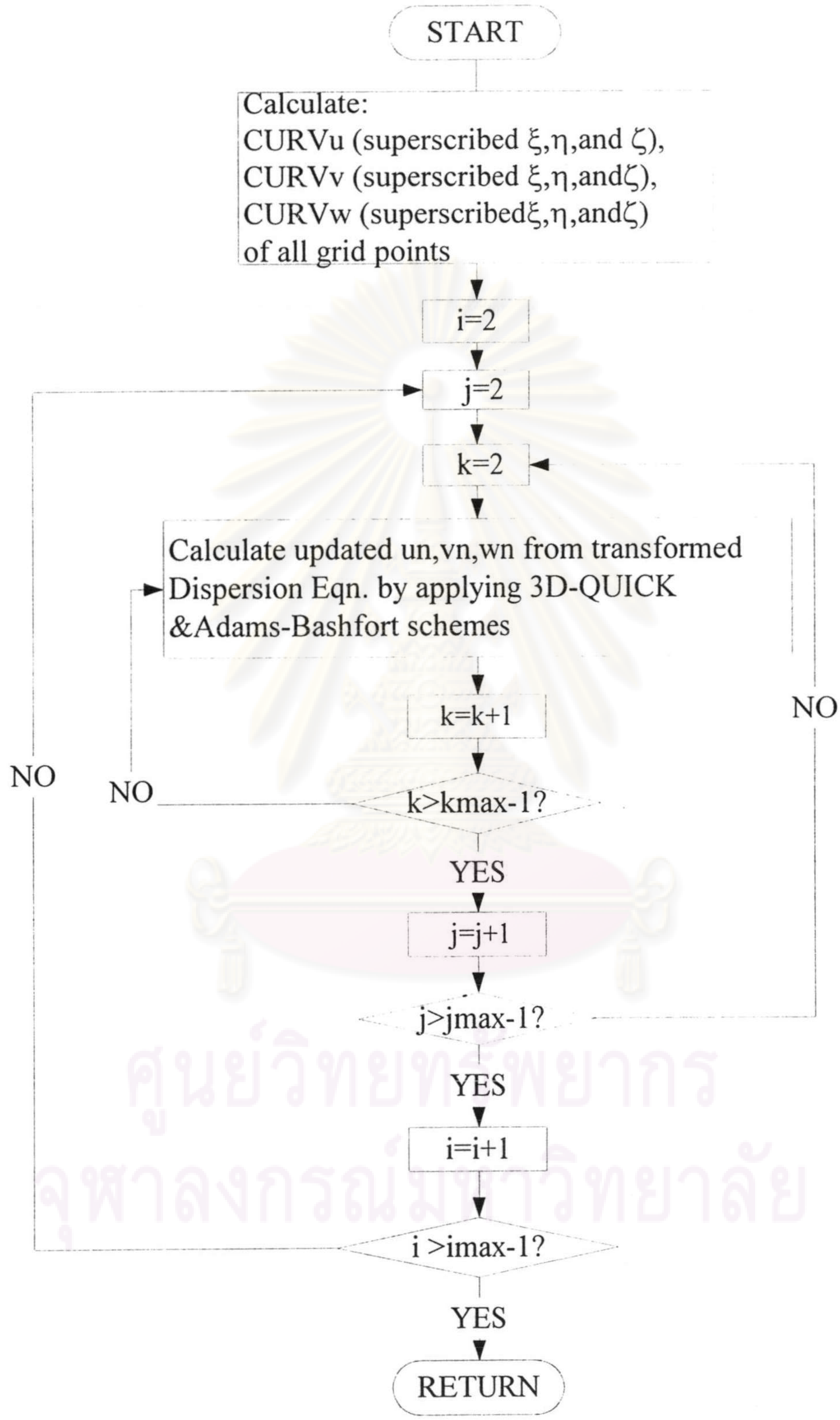
NA32PI SUBROUTINE



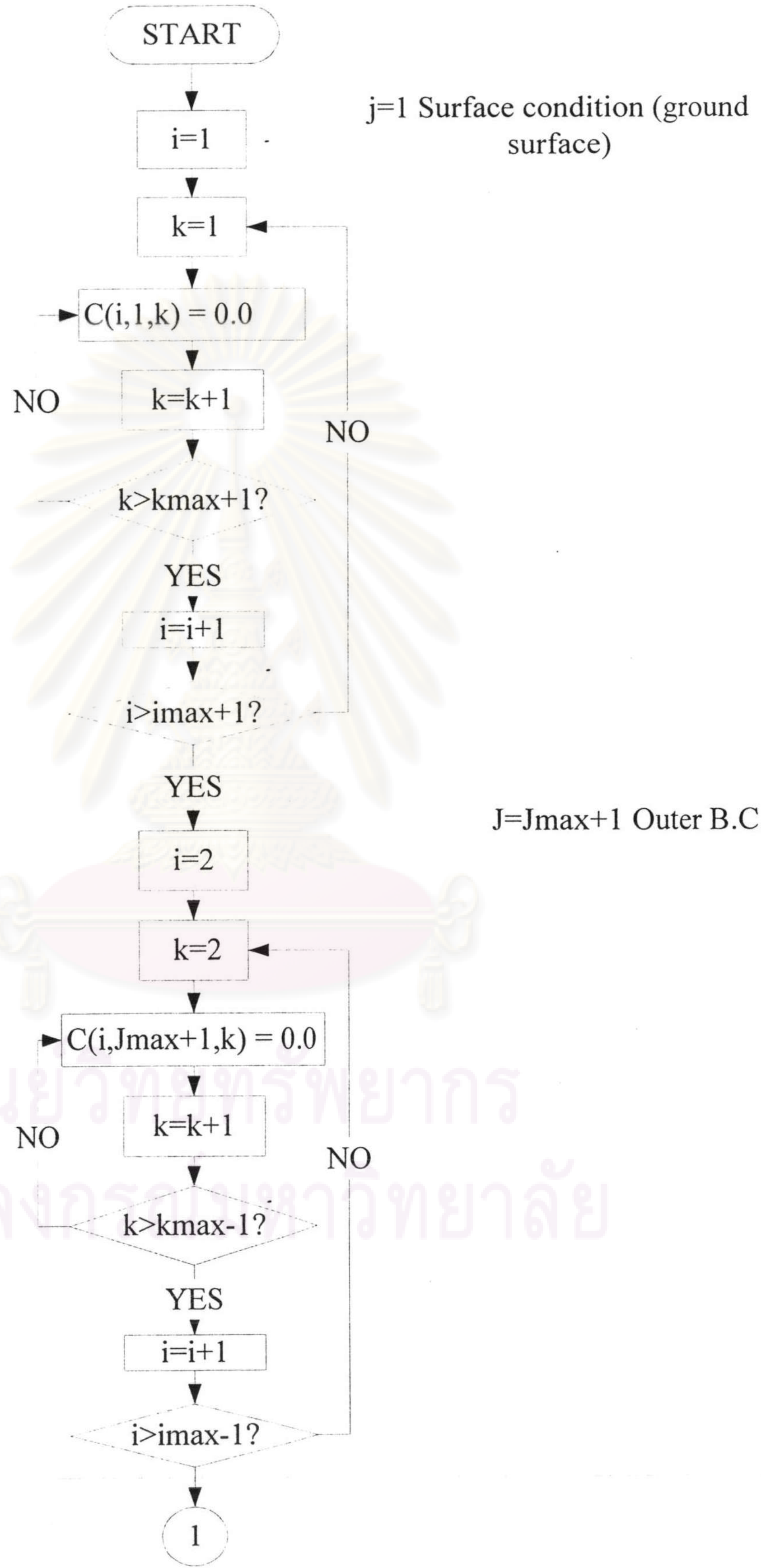
GKAKU3D (Dispersion Eq.)
Main Program



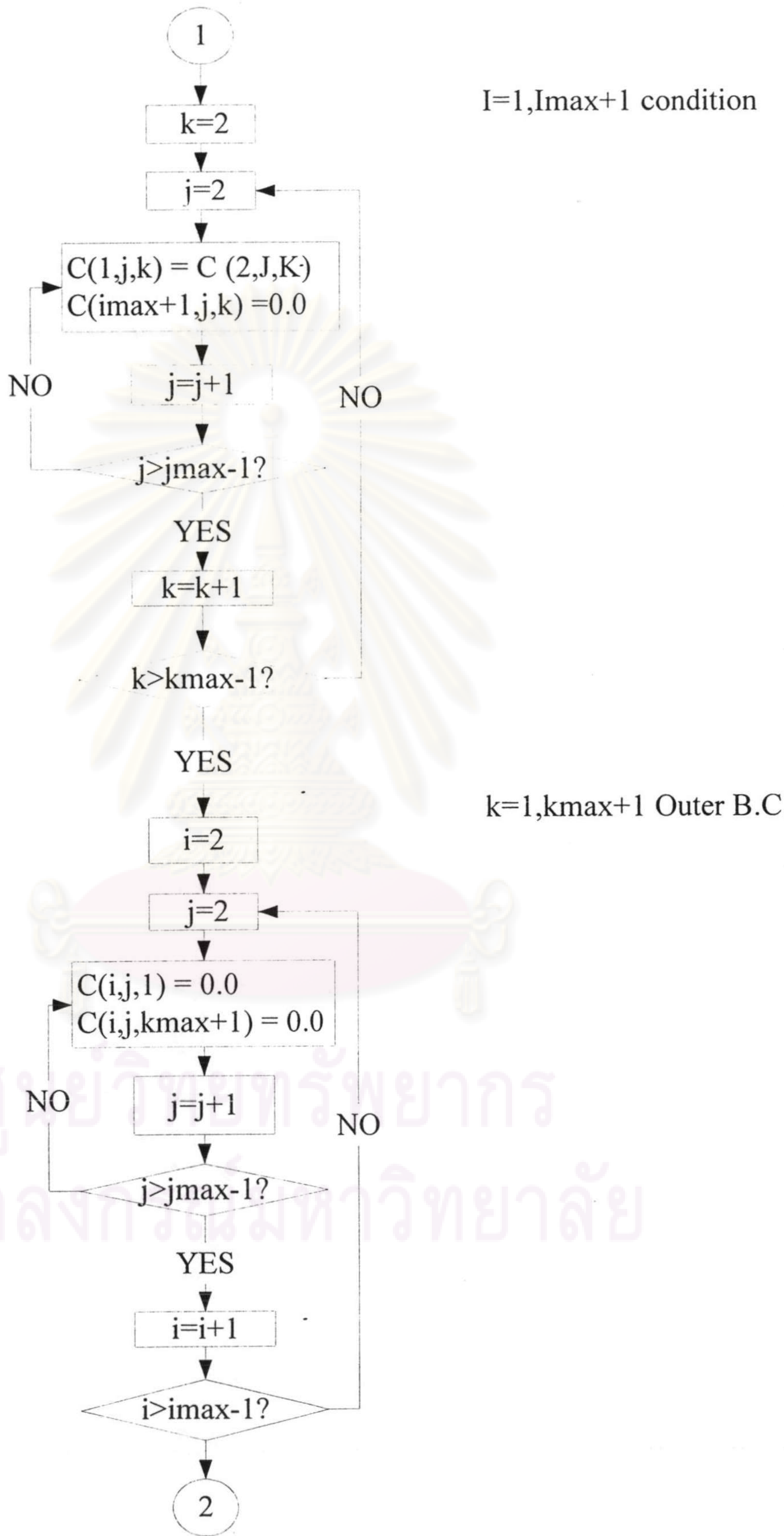
DIFFEQ SUBROUTINE



BOUND SUBROUTINE



BOUND SUBROUTINE (CON.)



BOUND SUBROUTINE (CON.)