由團塊群法研析農業微氣候之污染質散佈(二)微觀法

Contaminant Dispersal Analysis in Agromicroclimates Via Lump Grouping (II) Microscopic Approach

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摘 要

本文目的乃經由一微觀法之團塊群公式推導出一以動力反應及一度空間對流一擴散程序爲主之多種可反應污染質散佈理論。一線性第一階動力團塊可用來模擬可反應污染質質量傳輸現象。一度空間對流一擴散團塊則可用來模擬非完全混合之空間。本文亦詳論最後導得之系統方程式其特性及其穩定狀態與動態數值解技巧。模式之應用則選擇適當之農業微氣候系統做爲此微觀法理論之模式比對之依據。

關鍵詞：農業微氣候，動力團塊，一度空間對流一擴散團塊，微觀法。

ABSTRACT

The multiple, interactive contaminent dispersal theory is presented based upon a lump grouping formulation through the microscopic approach governed by the principle of kinetics and 1-D convection-diffusion processes. A linear first-order kinetics lump is introduced to model the interactive contaminant mass transport phenomena. A 1-D convection-diffusion lump is provided to model the imperfectly mixed zones. The character and solution of resulting system equations is discussed, and steady-state as well as dynamic numerical solution methods are also outlined. Appropriated agromicroclimate system models were selected to provide a computational impelentation and application of this microscopic approach.

Keywords: agromicroclimates, kinetics lump, 1-D convection-diffusion lump, microscopic approach.

INTRODUCTION

The macroscopic approach regarded to the contaminant dispersal analysis in an agromicroclimate of a farm structure has already been developed previously by author (Liao, 1992a). There exists two disadvantages when the macroscopic approach is being adopted: (1) it fails to account for the chemical dynamics of the agromicroclimates, and (2) it fails to describe the behavior of the imperfect zone lump. This paper attempted to study some of technical concerns by developing alternative modeling options based on lump grouping methodology from the viewpoint of microscopics that are designed to simulate both the multiple, interactive contaminant dispersal and imperfect mixed zone problems.

The theory and method presented are based upon a generalization of a farm structure idealization employed earlier (Liao, 1992a). Air flow system in agromicroclimates are idealized as groupings of mass transport lumps, rather than simply flow lumps are used previously, connected to discrete system nodes corresponding to well-mixed air zones within the agromicroclimate and its air duct work system. Equations governing contaminant dispersal in the whole air flow system due to air flow and reaction or sorption mass transport phenomena are formulated by grouping lump equations, in such a manner that the fundamental requirement of conservation of mass is satisfied in each zone.

In specific terms, the purposes of this paper are:

(1) To model the dispersal of interactive contaminant involving contaminant mass transport phenomena governed by basic principle of kinetics and introduces a linear first-order kinetics lump to achieve this end.

(2) To model hthe details of contaminant dispersal driven by covection-diffusion processes in one-dimensional flow situation (e.g., air delivering duct in mushroom growing houses) and introduces a convection-diffusion flow lump to achieve this end.

KINETICS LUMPS

Multiple-noninteractive Contaminant Dispersal

Air quality analysis in a farm structure environment will involve of several contaminants and their dispersal (Anderson et al., 1988; Liao and Feddes, 1991; Leonard et al., 1984; Groves and Ellwood, 1991). Some of these contaminants may: (1) be absorbed or adsorbed by building materials, or other contaminant particles, (2) settle from suspension or precipitate from gaseous solution, or (3) decompose chemically, or react with other contaminants to produce contaminants. Contaminant dispersal processes then can be characterized by the kinetics of: (1) sorption processes, (2) settiling or precipitation processes, or (3) chemical reaction processes.

The dispersal of each contaminant of a given set of noninteractive contaminants will be governed by the single-species contaminant dispersal equation, thus the dispersal of the noninteractive contaminant set may be represented by a set of the linear dynamic equations (Liao, 1992a):

$$[F^{\alpha}]\{C^{\alpha}\} + [M]\{dC^{\alpha}/dt\} = \{S^{\alpha}\}$$

$$[F^{\beta}]\{C^{\beta}\} + [M]\{dC^{\beta}/dt\} = \{S^{\beta}\} \qquad (1)$$

$$\cdots$$

where:

$\alpha, \beta, \ldots$ = species indices,

$\{C\}$ = species concentration vector, kg (kg of air)$^{-1}$,

$[F]$ = system mass flow matrix, kg m^{-3},

$[M]$ = system volumetric mass matrix, kg,

$\{S\}$ = species generation rate vector, kg hr^{-1}.

The uncoupled set of equations given by equation (1) may be expressed as an expanded system equation:

$$[F]\{C\} + [M]\{dC/dt\} = \{S\} \qquad (2)$$

The system flow transport matrix ([F]) may be first grouped by species (designed as "ρ") and then by lump (designed as "e") as:

$$[F] = \underset{e=a,b}{G} \left[\underset{\rho=\alpha,\beta}{G} [f^{e,\rho}] \right] \qquad (3)$$

where: G(·) is the grouping operator (Liao, 1992a).

The inner species grouping sum in equation (3) can be seen as a lump equation formulation for a noninteractive, multi-species flow lump i.e., the noninteractive, multi-species flow lump transport matrix. This multi-species flow lump could be grouped in the usual manner (Liao, 1992a) to form the system equations.

Reaction Kinetics

A general form of a chemical reaction involving reactants, α, β, ..., that react to form products, ρ, σ, ..., may be represented as (Moore and Pearson, 1981):

$$\alpha + \beta + ... \rightarrow \rho + \sigma + ... \tag{4}$$

Given the rate of change of a selected component's concentration, say α, is defined as:

$$R^{\alpha} = dC^{\alpha}/dt \tag{5}$$

The rate of change of the other components concentration may be related to that of the selected components as:

$$R^{\alpha} = (m^{\beta}/m^{\alpha})R^{\beta} = ... = -(m^{\sigma}/m^{\alpha})R^{\sigma} \tag{6}$$

where m^{α}, m^{β}, *and* m^{σ} is the relative masses of reactants and products. Thus the rate of a given chemical reaction may be described in terms of the rate of change of concentration of any one of the reactants and products.

Generally, the rate of a given chemical reaction may depend upon a variety of factors including reactant and catalyst concentrations, temperature (T) and pressure (P), and detailed mechanism of the chemical reaction, therefore, rate expression take the general functional form as,

$$R^{\alpha} = R^{\alpha}(C^{\alpha}, C^{\beta}, ..., C^{\rho}, C^{\sigma}, ..., T, P, ...) \tag{7}$$

In some instance the rate of reaction may remain more or less constant: $R^{\alpha} = R_{o}^{\alpha}$, or depend only on temperature and pressure: $R^{\alpha} = R_{o}^{\alpha}(T, P)$. Examples include the catalytic decomposition of some gases, such as NH_3 in pig houses (Liao, 1992b), the controlled burning of fossil fuel in agricultural machinery plants (Hinz, 1989), and other relatively slow reaction driven by reactant and product concentrations that remain, more or less, constant over the time of interest.

Rate expression for certain general classes of reactions, inlcuding single-reactant, consecutive, reversible, and paralledl first-order reaction (Moore and Pearson, 1981), often take the form of linear combination of contaminant concentration:

$$\{R\} = -[k]\{C\} + \{R_{o}\} \tag{8}$$

where $[k]$ may be referred to as the rate coefficient matrix, and can be expressed:

$$[K] = \begin{bmatrix} K^{\alpha\alpha} & -K^{\alpha\beta} & \cdots & -K^{\alpha\sigma} \\ -K^{\beta\alpha} & K^{\beta\beta} & \cdots & -K^{\beta\sigma} \\ \cdots & \cdots & \cdots & \cdots \\ -K^{\sigma\alpha} & -K^{\alpha\beta} & \cdots & K^{\sigma\sigma} \end{bmatrix} . \tag{9}$$

It is possible to linearlize any given rate expression about some state of concentration, say $\{C_{o}^{\alpha}, C_{o}^{\beta}, ...\}$, by employing a Taylor's expansion about that state to obtain an approximate rate expression expressed as the sum of a series of first-order rate expressions as:

$$R^{\alpha}(C^{\alpha}, C^{\beta}, ...) = R^{\alpha}(C_{o}^{\alpha}, C_{o}^{\beta}, ...) + \partial R^{\alpha}(C_{o}^{\alpha}, C_{o}^{\beta}, ...)/\partial C^{\alpha}(C^{\alpha} - C_{o}^{\alpha}) + \partial R^{\alpha}(C_{o}^{\alpha}, C_{o}^{\beta}, ...)/\partial C^{\beta}(C^{\beta} - C_{o}^{\beta}) + ... \tag{10}$$

Then, equations (10) together with equation (6) can be used to form a linearlized system of first-order rate expression: equation (8).

Linear systems of first-order reaction expression are defined by the characteristics of their reaction rate coefficient matrix ($[K]$).

Kinetics Lump Equations

The development of a general kinetics lump equation is straightforward. Limiting the consideration to mass transport phenomena occurring within a specific zone "i", containing a set of contaminant species, α, β, γ, ..., the relevant lump variables can be first expressed as:

$$\{C^e\} = \{C_i^{e,\alpha}, C_i^{e,\beta}, C_i^{e,\gamma}, ...\}^T \quad (11)$$

and

$$\{w^e\} = \{w_i^{e,\alpha}, w_i^{e,\beta}, w_i^{e,\gamma}, ...\}^T \quad (12)$$

where: $\{w^e\}$ is lump species mass flow rate (kg hr^{-1}).

Assuming that the mass transport phenomena to be modelled is governed by the kinetics discussed above, a general kinetics lump equation follows directly from the definition of rate of reaction (equation (5)) and the general form of rate expressions (equation (8)) as:

$$\{w^e\} = -[M_i^e]\{R_i^e(\{C_i^e\}, T, P)\} \quad (13a)$$

where:

$$[M_i^e] = diag\,[M_i, M_i, ..., M_i] \quad (13b)$$

$$[R_i^e(\{C_i^e\}, T, P)] \equiv \{R_i^\alpha(C_i^{e,\alpha}, C_i^{e,\beta}, ..., T, P), R_i^\beta(C_i^{e,\alpha}, C_i^{e,\beta}, ..., T, P), ...\}^T \quad (13c)$$

For reaction kinetics described by systems of first-order equations (equation (8)).

$$\{R_i^e(\{C_i^e\}, T, P)\} = -[k_i^e]\{C_i^e\} + \{R_{oi}^e\} \quad (14)$$

The kinetics lump equation (13) becomes:

$$\{w^e\} = [M_i^e][k_i^e]\{C_i^e\} - [M_i^e]\{R_{oi}^e\} \quad (15)$$

It will be convenient to introduce a new variable for the linear first-order lump kinetics transport matrix ($[K_i^e]$) as:

$$[K_i^e] \equiv [M_i^e][k_i^e] \quad (16)$$

and a corresponding variable for the system kinetics transport matrix, [K], that is grouped from the lump kinetics transport matrices in the usual manner, as:

$$[K] = \underset{kinetics\ lump}{G} [k^e] \quad (17)$$

Therefore, the system ttansport matrix ([W]) can be expressed by the sum of the system flow matrix ([F]) and the system kinetics transport matrix ([K]) as:

$$[W] = [F] + [K] = \underset{flow\ lumps}{G} [f^e] + \underset{kinetics\ lumps}{G} [k^e] \quad (18)$$

CONVECTION-DIFFUSION LUMPS

In some situations the analyst may be interested in the details of dispersal in some flow passage or may feel the noninstantaneous nature of the flow should not be ignored. If flow in these flow passage may be assumed to be practically one-dimensional (e.g., longer portions of air duct works in mushroom houses and greenhouses) then the details of the convection and diffusion mass transport processes that driven the dispersal may be accounted for using groupings of two-node convection-diffusion lumps.

The convection-diffusion equation is often expresses in dimensionless form as (Nauman and Buffham, 1983):

$$1/P_e\,\partial^2 C/\partial X^2 + \gamma = \partial C/\partial \tau + \partial C/\partial X \quad (19a)$$

in which:

$$P_e \equiv w^e L/(\rho A D^\alpha) = \bar{\mu} L/D^\alpha \quad (19b)$$

where:

P_e = dimensionless Peclet number,

X = dimensionless length = x/L,

τ = dimensionless time = $t/\bar{t}$,

γ = dimensionless generation rate = gL/w^e,

$\bar{t}$ = nominal transit time = $L/\bar{u}$, hr,

$\bar{u}$ = bulk fluid velocity = $w^e/(\rho A)$, m hr^{-1},

ρ = fluid density, kg m^{-3},

D^α = dispersal coefficient for one species, m^2 hr^{-1},

L = length of tee flow passage, m,

g = species generation rate per unit length of passage, kg hr^{-1} m^{-1}.

The Peclet number characterizes the convection-diffusion process in a flow passage not involving a kinetic rate expression. It provides a meaure of the importance of convection mass transport relative to diffusion mass transport.

The dispersal coefficient is reasonably correlated to the characteristic Reynolds number (R_e) of the flow and is practically independent of species molecular diffusivity as indicated by the Taylor expression (Wen and Fan, 1975):

$$D^\alpha \approx D^\beta \approx \ldots \equiv D = 2\bar{u}R(3.0\text{x}10^7/R_e^{21} + 1.35/R_e^{0.125}); \quad R_e > 2000 \tag{20}$$

where: R is the flow passage radius (m); $R_e \equiv 2\rho\bar{u}R/\mu$; the Reynolds number; μ is the flow fluid viscosity (kg hr^{-1} m^{-1}).

CONVECTION-DIFFUSION EQUATIONS

Finite element solution of convection-diffusion equation of the form of equation (19) have received considerable attention in recent years. Following the one-dimensional example discussed by Huebner and Thornton (1982), lump equation (19) using linear shape functions (i.e., assuming species concentration vary in a piecewise linear manner along the flow passage) and applying either the convectional Galerkin method or the upwind Retrov-Galerkin method in the formulation of these lump equations. The resulting lump equation are (Huebner and Thornton, 1982; p. 448):

$$\{w^e\} = [[f_c^e] + [f_d^e]]\{C^e\} + [m^e]\{dC^e/dt\} - \{g^e\} \tag{21a}$$

where:

$$\{w^e\} = \{w_i^e, w_j^e\}^T$$

$$\{C^e] = \{C_i^e, C_j^e\}^T$$

$$[f_c^e] = w^e/2 \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \phi w^e/2 \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{21b}$$

(the convection component of the lump flow transport matrix),

ϕ = so-called upwind parameter, $0 \leqslant \phi \leqslant 1$,

$$[f_d^e] = \rho AD/L^e \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{21c}$$

(the diffusion component of lump flow transport matrix),

L^e = the length of the lump,

$$[m^e] = \rho AL^e/6 \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \phi\rho AL^e/4 \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix} \tag{21d}$$

(the lump volume mass matrix),

$$\{g^e\} = gL^e/2 \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \phi gL^e/2 \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} \tag{21e}$$

(the internal generation rate vector),

for total fluid mass flow rate (w^e) through the flow passage from node i to node j.

The convection-diffusion equation defined by equation (21) may be grouped along with the simple flow lump equation and kinetics lump equations to form the system equations. The convection-diffusion lump introduces, however, nondiagonal contributions to the system mass matrix ([M]) that adds some complexity to the grouping and solution algorithms used in the computational implementation of the contaminant dispersal theory. To avoid this complexity one may replace the so-called consistent lump volume mass matrix (equation (21d)) with a diagonal grouped mass approximation to it, which is given by Huebner and Thornton, 1982; p. 416):

$$[m^e] = \rho AL^e/2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{(lumped)} \qquad (22)$$

Steady-State Analysis. When considering steady-state flow without internal generation, Huebner and Thornton (1982) show that instability may be avoided if an upwind parameter is selected satisfying the condition;

$$\phi \geqslant 1 - 2/P_e^e; \quad P_e^e > 2$$

$$\phi = 0; \quad P_e^e \leqslant 2 \qquad (23)$$

where P_e^e is the lump Peclet number ($P_e^e \equiv w^e L^e/(\rho AD) = \bar{u}L^e/D$).

For this problem the convection-diffusion equation simplifies to:

$$1/P_e d^2C/dX^2 = dC/dX \qquad (24a)$$

which may be solved for the boundary conditions:

$$C(x=0) = C_o; \quad C(x=L) = 0 \qquad (24b)$$

to obtain an exact solution:

$$C(x/L)/C_o = (exp(P_e/L(x/L)) - exp(P_e/L))/$$

$$(1 - exp(P_e/L)); \quad 0 \leqslant x/L \leqslant 1 \qquad (25)$$

that will be compared to approximate solution obtained using convection-diffusion lumps. The results clearly show that the numerical instability that may result when upwinding is not used for high lump Peclet numbers (Huebner and Thornton, 1982).

Dynamic Analysis: In dynamic analysis, accuracy is affected not only by lump size, and the degree of upwinding chosen, but also by the integration step selected to complete the dynamic solution. For different Peclet numbers, three alternatives can be obtained.

(1) For P_e=0 the duct becomes a well-mixed system, the initial condition throughout the duct becomes $(1/(\rho AL))$, and the outlet concentration decays exponentially:

$$C(L,t)/(1/\rho AL)) = exp(-t/\bar{t}); \; P_e = 0 \qquad (26)$$

(2) For relatively large Peclet numbers the outlet concentration is well approximated by the following expression reported by Nauman and Buffham (1983):

$$C(L,t)/(1/(\rho AL)) = \left(P_e/(4\pi(t/\bar{t})^3)\right)^{1/2}$$

$$exp\left(-P_e(1 - t/\bar{t})^2/(4t/\bar{t})\right); \; P_e > 16 \quad (27)$$

(3) For vary large Peclet numbers the outlet conventration approaches a Gaussian distribution (Wen and Fan, 1975):

$$C(L,t)/(1/\rho AL) = (P_e/4\pi)^{1/2}$$

$$exp\left(P_e(1 - t/\bar{t})^2/4\right); \; P_e \gg 16 \qquad (28)$$

In all cases the upwind parameter was chosen to satisfy the lower bound of the stability requirement of equation (27).

Analytical Properties: The numerical properties of the convection-diffusion flow lump have been seen to be dependent upon the lump Peclet number. To investigate this dependency in greater detail, equations (25b) and (25c) may be rewritten in terms of the lump Peclet number, as:

$$[f^e] = [[f_c^e] + [f_d^e]]$$

$$= w^e/2 \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \phi w^e/2 \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$+ \rho DA/L^e \begin{bmatrix} 1 & -1 \\ -1 & \end{bmatrix}$$

$$= w^e/2 \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + (\phi + 2/P_e^e) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (29)$$

The stability requirement of equation (23) may be rewritten as:

$$\phi + 2/P_e^e \geqslant 1; \quad P_e^e > 2$$

$$\phi = 0; \; P_e^e \leqslant 2 \quad (30)$$

Assume that the flow transport matrix will be an M-matrix: a real square matrix with positive diagonal elements and nonpositive off-diagonal elements such that $[[f^e] + \xi[I]]$ is strictly diagonally dominant for all $\xi < 0$. It was shown earlier (Liao, 1992a) that lump flow transport matrices satisfying this condition (coupled with mass matrices that are positive diagonal matrices) lead to system transport matrices are nonsingular.

Tanks-in-Series Idealizations: In the chemical engineering literature the so-called tanks-in-series idealization is frequently employed to model the behavior of one-dimensional convection-diffusion transport processes or other processes whose inlet-outlet transformation characteristics appear to match those described by one-dimensional convection-diffusion equation (Nauman and Buffham, 1983). In the tanks-in-series idealization a portion of the flow (θ) assumed to recirculate between adjacent tanks is used to model the nature of turbulent and molecular diffusion (Nauman and Buffham, 1983).

The subgrouping of this tanks-in-series idealization consisting of half of two adjacent unit tanks and the connecting simple flow lumps (Figure 1), which it shall be referred to as a tanks-in-series lump, may be compared directly to the convection-diffusion flow lump.

Lump equations for the tanks-in-series flow lump may be grouped directly from the simple flow equations:

$$\{w^e\} = [f_t^e]\{C^e\} + [m^e]\{dC^e/dt\} \quad (31a)$$

where:

$$[f_t^e] = w^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} + \theta w^e \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (31b)$$

(tanks-in-series flow lump transport matrix). Comparing these equation (31) with the convection-diffusion lump equation (equation (21)), it can be seen that they become equivalent when,

$$\theta = \rho AD/(w^e L^e) = 1/P_e^e \quad (32)$$

and a full upwinding ($\phi = 1.0$) is used.

In comparing the convection-diffusion lump and the tanks-in-series idealization, modeling high Peclet number flows will demand a fine subdivision of lumps and modeling low Peclet number flows will not (Nauman and Buffham, 1983). By choosing different Peclet numbers, the convection-diffusion lump may be used to model a zone that is not perfectly mixed. Therefore, the convection-diffusion lump developed to model flow transport situations become apparent that this lump provides one means to model imperfectly mixed zones.

Therefore, two aspects of the convection-diffusion lump are especially important: (1) the convection-diffusion lump is based upon a microscopic description of dispersal (i.e., it is based upon partial differential mass balance relations) and its use provides a first example of combining macroscopic modeling methods (i.e., the well-mixed zone and simple flow lumps (Liao, 1992a)) with microscopic methods in a single analytical procedure; and (2) from another perspective an one-dimensional flow regime may be thought to represent an imperfectly mixed zone, thus, the convection-diffusion flow lump may be considered to be an imperfectly mixed zone lump.

IMPLEMENTATION AND APPLICATION

An Agricultural Machinery Plant Model

Detailed field investigation of an agricultural machinery plant measuring CO, NO, NO_2 emission characteristics of the burning of fuel within the plant and the dispersal of these contaminants throughout the plant under a variety of different weather conditions was already reported by Hinz (1989). Figure 1 illustrates an idealized lump flow model of the plant. Figure 2 shows the range of the principal pollutant sources. Table 1 lists the system parameters used in this model simulation.

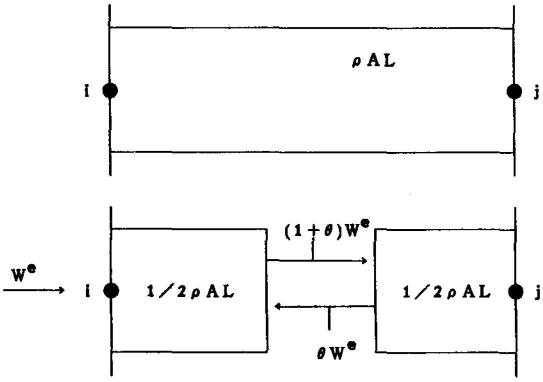

Fig. 1. The equivalence of the lump convection-flow and a tank-in series lump.

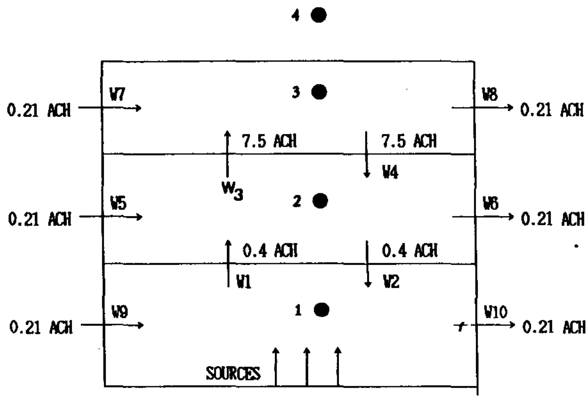

Fig. 2. An agricultural machinery plant idealization: a 4-node lump model.

Table 1. System parameters used in model simulation for an agricultural machinery plant (Hinz, 1989)

Air volume: $V_1 = V_2 = V_3 = 126.5\ m^3$, $V_4 = 126.5 \times 10^9\ m^3$.
Air density = 1.2 Kg m^{-3} (@ 1 atm 25°C)
Local air flow rate: $W_1 1 = W_2 = 0.4 \times 126.5 \times 1.2 = 60.72$ Kg hr^{-1}; $W_3 = W_4 = 7.5 \times 12.65 \times 1.2 = 1138.5$ Kg hr^{-1}; $W_5 = ... = W_{10} = 0.21 \times 126.5 \times 1.2 = 31.88$ Kg hr^{-1}
Steady-state source emission rate: S(s,s) NO_2 = 1.80 mg min^{-1}; CO = 14.7 mg min^{-1}; NO = 2.55 mg min^{-1}

The instantaneous emission rate, S(t), is plotted relative to the steady-state value, S(s,s). The NO_2 emission characteristics were more or less constant and are not illustrated. NO_2 is a reactive contaminant and was modeled as using the measured reactivity of k = 2.4 hr^{-1} (Borrazzo et al., 1987): $d[NO_2]/dt = -k^{NO_2}[NO_2]$, where: $[k] = [k^{NO_2}] = 2.4 hr^{-1}$.

Figures 4 – 6 show the short-time responses of dispersal of NO_2, CO, and NO in a 4-node lump idealization for a agricultural machinery plant. In this particular case, it was assumed that the measured whole-building fresh air infiltrated rate of 0.21 air exchanges per hour (ACH) was distributed equally in all these zone, the first-to-second lump local airflow rate was assumed to be 0.4 ACH, the second-to-third lump local airflow rate was assumed to be 7.5 ACH, and all airflow rates were assumed to be constant.

Convection-Diffusion Lump Model

Case 1: Steady-state condition.

Consider the problem: The dispersal of a contaminant along a straight flow passage under steady-state flow conditions, without generation, and with inlet contaminant concentration maintained at C_o and outlet concentration maintained at zero (Figure 7). For this problem the convection-diffusion equation used is equation (25), that will be compared to approximate solutions obtained using convection-diffusion lump model.

For the approximate solution, an idealization consisting of a series of ten convection-diffusion flow lump is considered (Figure 7). The solution generated for two Peclet numbers, $P_e = 0.2$ and $P_e = 20$; and two upwinding factors, $\phi = 0.0$ and $\phi = 1.0$. The exact with the approximate solutions are compared in Figure 8.

The results show that the numberical instability may result when upwinding is not used for high Peclet number. For convection-dominated flow, which should be expected to be typical in building HVAC ductwork under operating conditions (ASHRAE, 1985), and therefore that a fine subdivision o a given duct or employ upwinding to maintain numerical stability may be adopted.

Case 2: Dynamic condition.

Consider the problem: Fluid flows through a duct of length L and radius R at a mass flow rate W^e, a contaminant is injected into the inlet stream at a rate S(t) for a short time interval introducing a pulse of contaminant of mass 1 into the inlet stream; the pulse is convected and dispersed as it moves along the duct (Figure 9). The objective is to determine the concentration time history of the contaminant as it emerges from the outlet of the duct.

The exact solution to this problem is available for an impulse (i.e., a pulse defined by the dirac delta function), for closed inlet and outlet conditions, and already derived in equations (30) – (32) for different Peclet number.

Approximate solutions to this problem were computed using a 12-node with 10-lump subdivision (Figure 9). The closed boundary condition was modeled using the simple flow lump as this lump models (completed-mixed) plug flow conditions as required. The impulse was approximated by a pulse of finite but small duration. In all runs the upwinding parameter was chosen to satisfy the lower bound of the stability of equation (23). The results are compared and shown in Figure 10.

In is seen that the approximate solution for the low Peclet number ($P_e = 1$) approaches the exact well-mixed solution. A comparison of the results of the 10-lump model approximation for $P_e = 10$ indicates that a convergent solution was obtained, yet when this result is compared to the exact results reported by Wen and Fan (equation (45)) (1975) the amplitude appears to be underestimated by about 10% (Figure 10). This same comparison for $P_e = 20$ indicates that a convergent solution was almost but not quite achieved.

An additional subdivision would presumably reveal convergence, and the error in amplitude estimation was approximately 20% (Figure 10). It is interesting to note that the lump Peclet number for these two convergence solutions: 10-lump solution at $P_e = 10$ and the 20-lump solution at $P_e = 20$, are both equal to 1.0; a condition that demands no upwinding ($\phi = 0$) to maintain numerical stability.

The study for $P_e = 20$ corresponds to studying the transport of a pulse through a circular duct for 1 m radius having a length of 10 m with a bulk flow velocity 2 m s^{-1}. For these conditions, the dispersal coefficient may be expected to be about 1 m^2 s^{-1} (ASHRAE, 1985). The results (Figure 10) were computed using a pulse

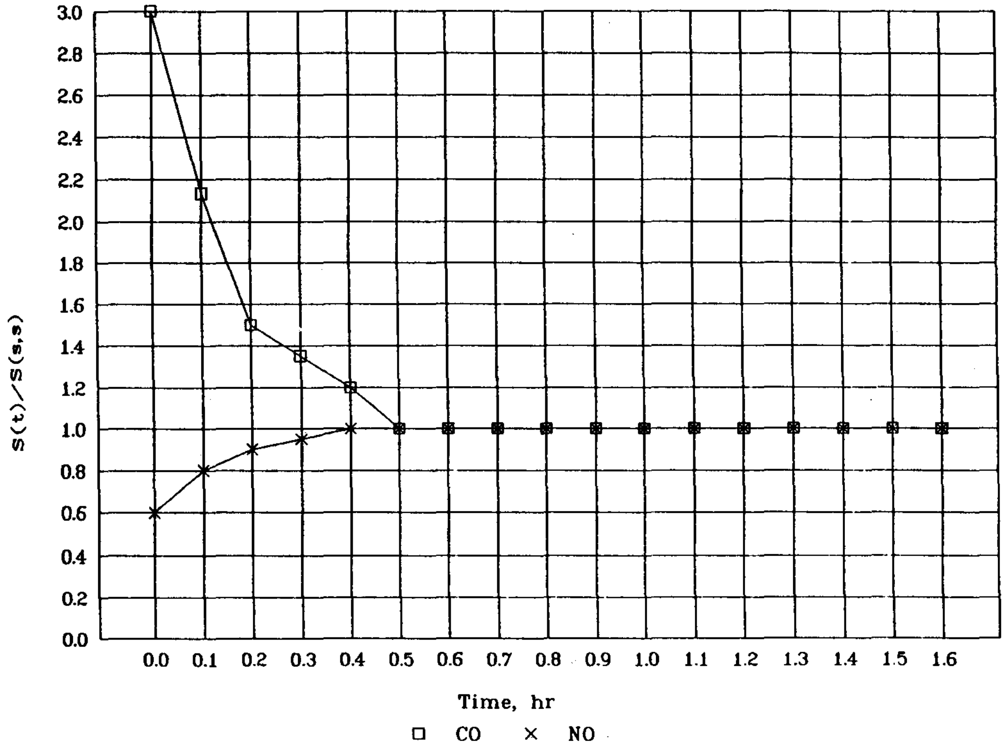

Figure 3. Time evolution of contaminant source emissions of CO and NO concentrations

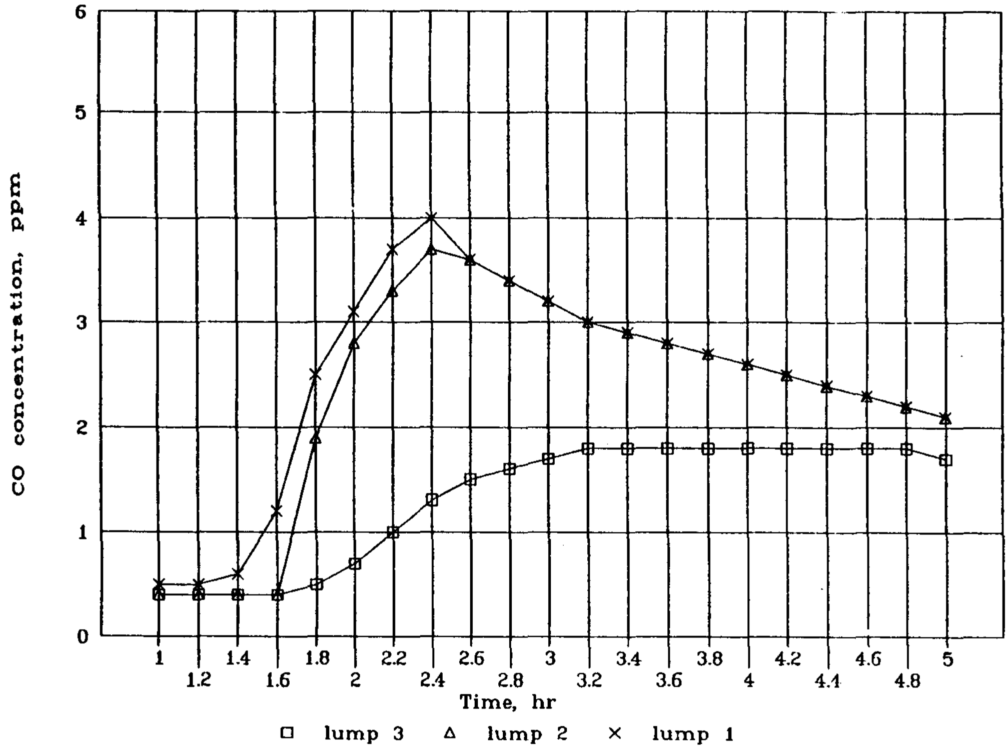

Figure 4. Short-time change of contaminant dispersal for CO concentration in a 4-node lump model

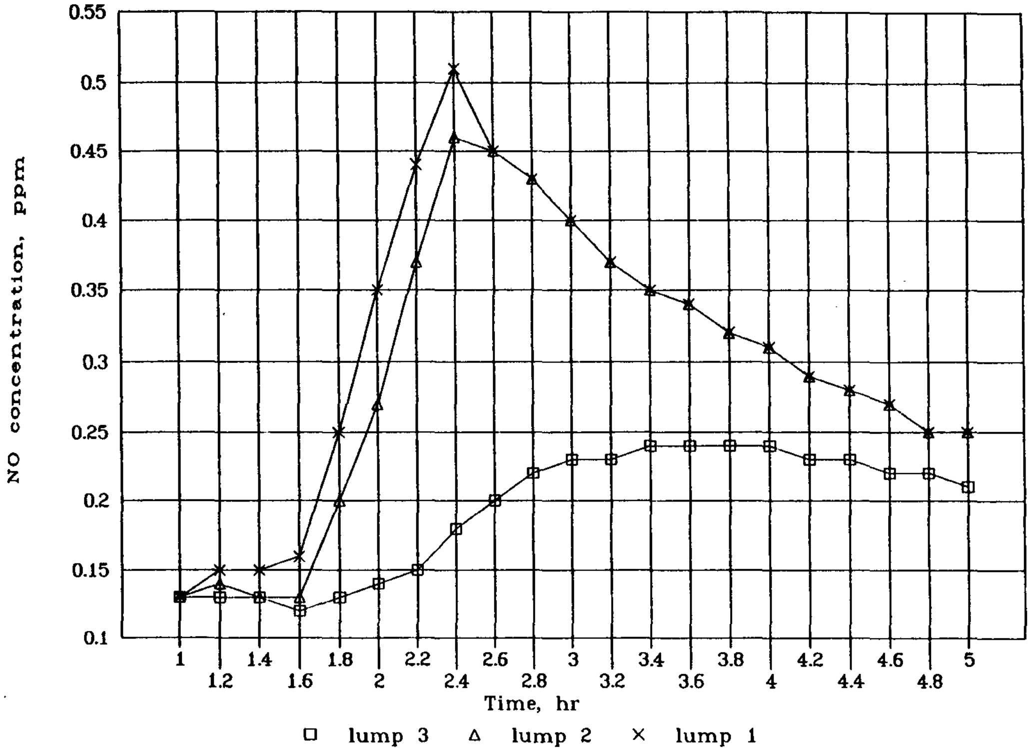

Figure 5. Short-time change of contaminant dispersal for NO concentration in a 4-node lump model

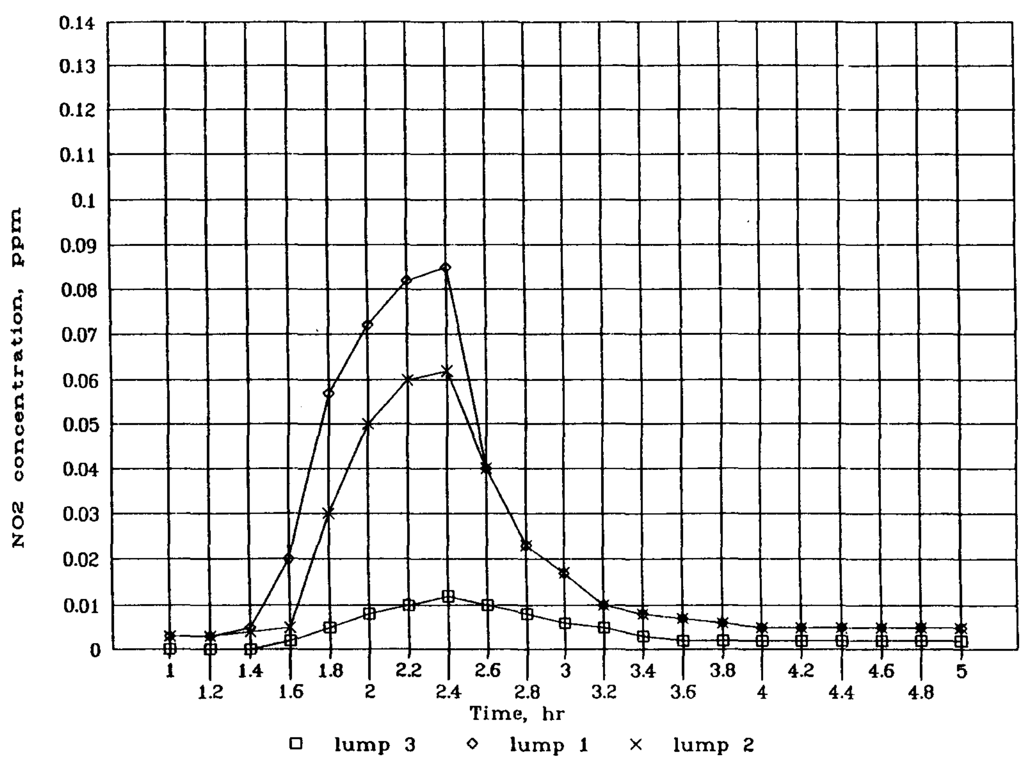

Figure 6. Short-time change of contaminant dispersal for NO_2 concentration in a 4-node lump model

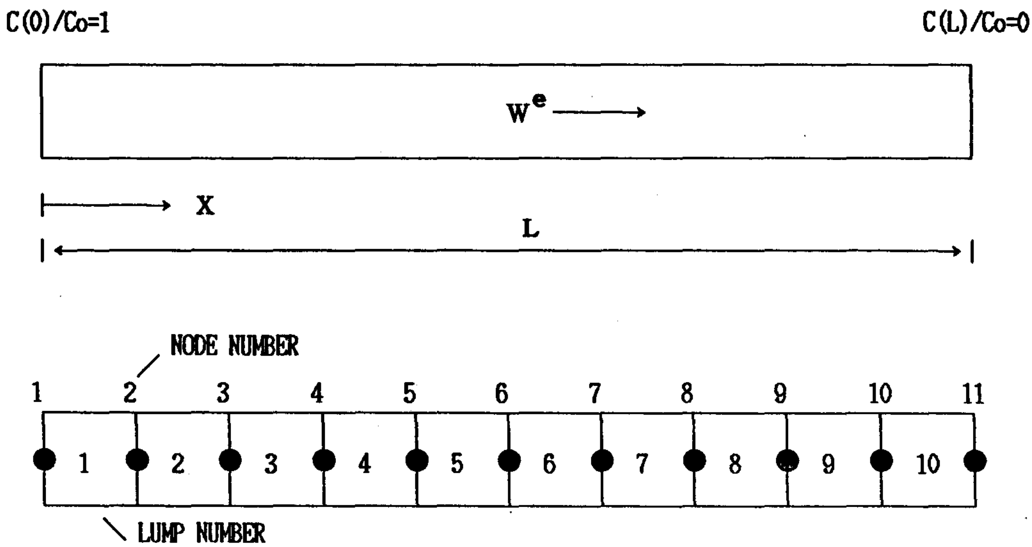

Figure 7. Steady-state convection-diffusion example and corresponding 10-lump idealization

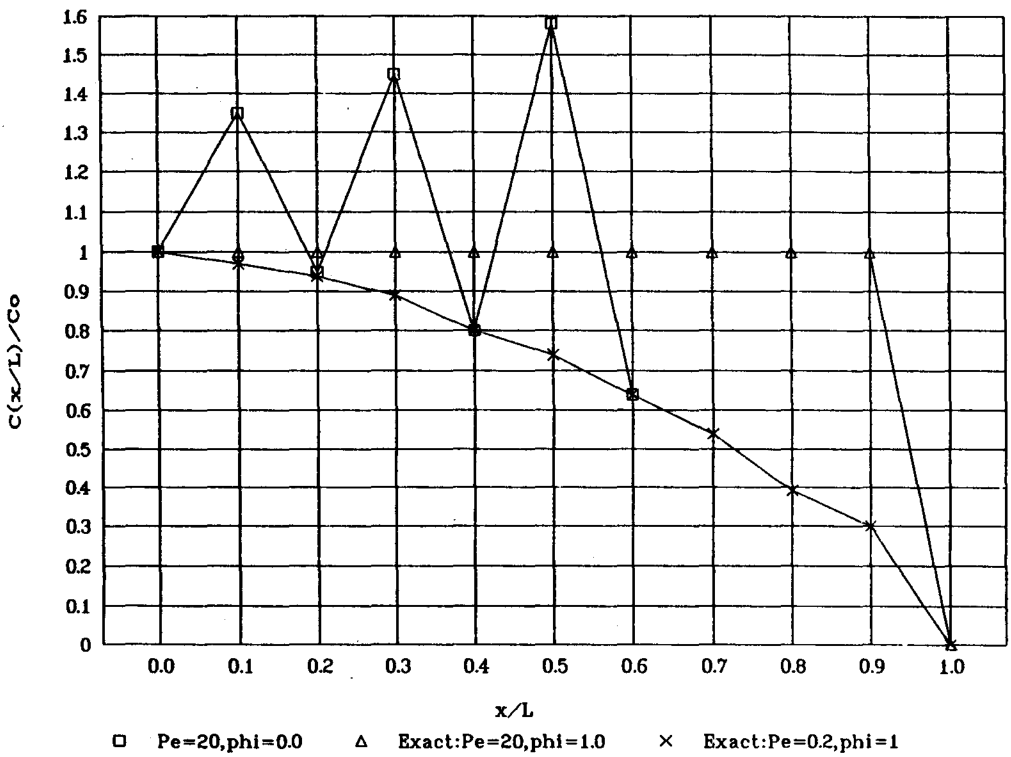

Figure 8. Comparison of exact and lump model solutions for a steady-state convection-diffusion model

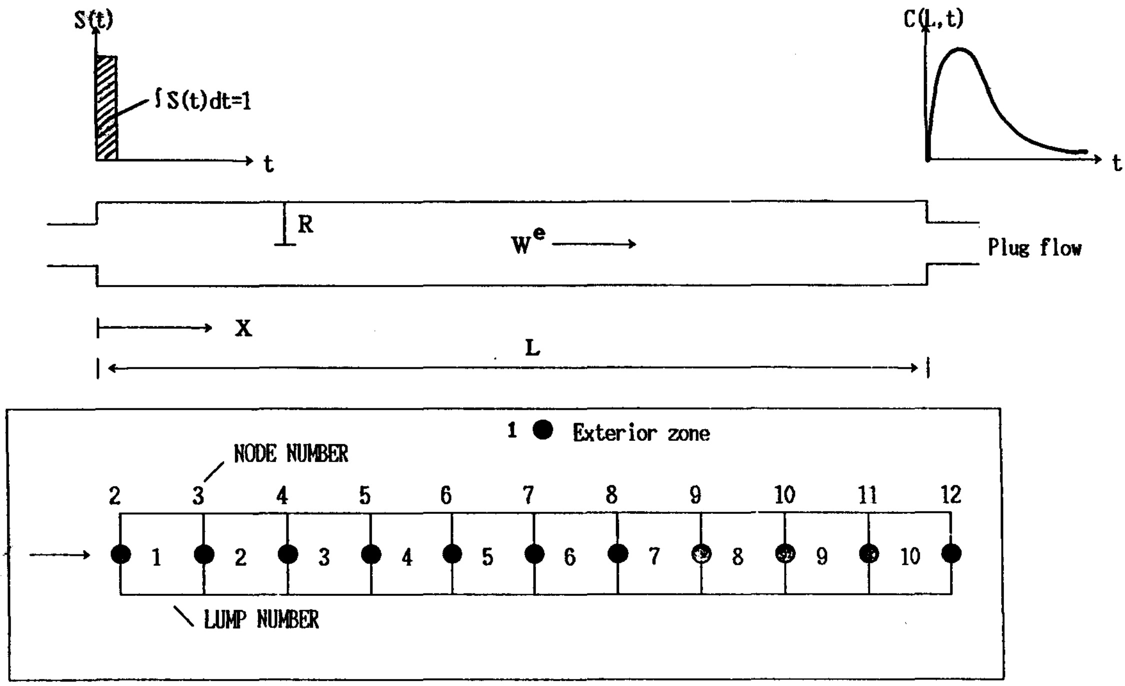

Figure 9. The transport of an impulse in a duct and the corresponding 10-lump idealization

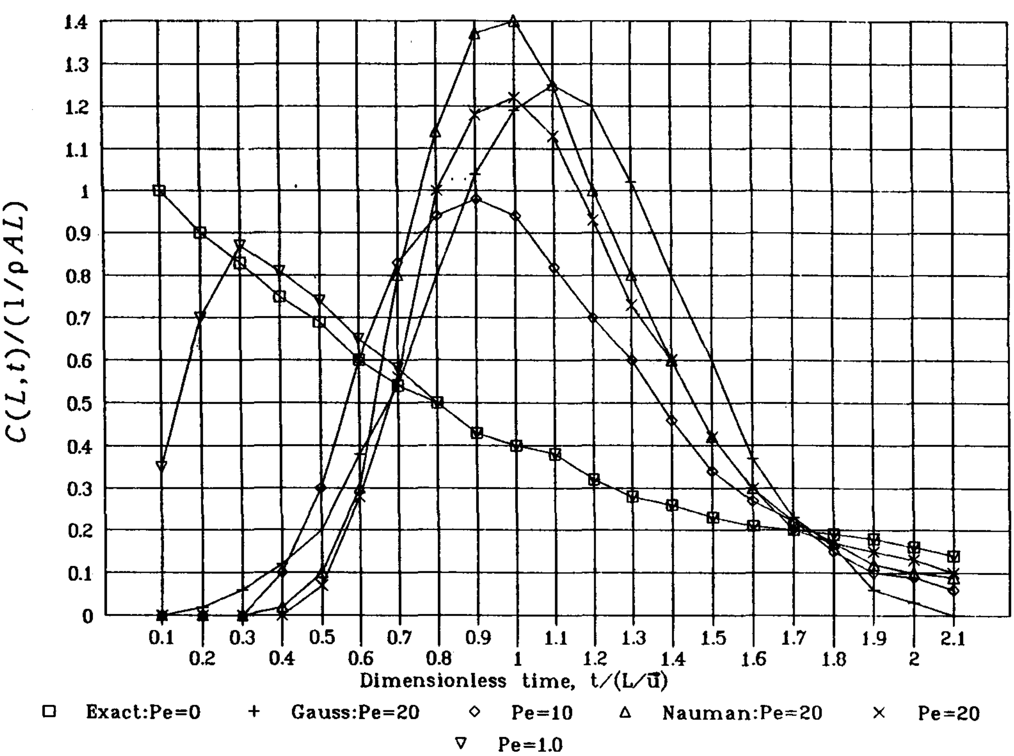

Figure 10. Comparison of analytical solutions with lump model solutions for dynamic convection-diffusion model

duration of 0.005 sec (i.e., the pulse duration, say 0.001 times the nominal transit time: $\bar{t} = L/\bar{u} = 10m/2ms^{-1} = 5$sec.). In order to gain the short-time pulse accurately and to achieve a convergent solution, the dynamic solution was computed using a time step of 0.001 sec.

In practical situations the inaccuracies revealed in these studies are likely to be considered very small, thus, the convection-diffusion flow lump should provide a practically useful analytical tool. This studies also suggest that when employing convection-diffusion lumps in an idealization of a agromicroclimate airflow system, it is very likely that extremely small time step will be required to obtain a convergence solution.

SUMMARY AND CONCLUSIONS

1. In the first part of this paper, a clearer definition of contaminant dispersal analysis in agromicroclimates has already been given based upon a lump grouping formulation of the well-mixed zone simplification of the macroscopic equations of motion. The noninteractive contaminant dispersal theory presented in the first part of this project has been extended in this part through: (1) the introduction of lump equations that may be used to model mass transport phenomena governed by first-order kinetics, and (2) through the introduction of lump equations that may be used to model the details of mass transport driven by convection and diffusion processes in one-dimensional flow paths.

2. Although it is well recognized that kinetics plays an important role in chemical sorption, and settling processes that affect contaminant dispersal processes in agromicroclimates, the detailed knowledge needed to apply kinetics analysis techniques presented here is often not available and actual field or experimental measured data needed to validate any modeling effort is scarce. Thus, the application of the kinetics techniques presented here has become an area emphasis in the recommendation for future research.

3. It was recognized that the 1-D convenction-diffusion lump can provide one means to model the imperfectly mixed zones. Thus, this mass transport lump could be considered to be a imperfectly-mixed zone lump. In this new formulation, the well-mixed model becomes one special case and a framework is provided for the development of other imperfectly mixed zone lumps.

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REFERENCES

1. Anderson, G. A., R. J. Smith, D. S. Bundy, and H. C. Hammond. 1987. Model to predict gaseous contaminants in swine confinement buildings. J. Agric. Engng Res. 37 (4): 235-253.
2. ASHRAE. 1985. ASHRAE handbook of fundamentals. American Society of Heating, Refrigeration, and Air Conditioning Engineers, New York, NY.
3. Borrazzo, J. E., J. F. Osborn, R. C. Fortmann and C. C. Davidson. 1987. Modeling and monitoring of CO, NO and NO_2 in a modern townhouse. Atmosph. Environ. 21. 229-311.
4. Groves, J. A., and P. A. Ellwood. 1991. Gas in agricultural slurry stores, Ann. Occup. Hyg. 35 (2): 139-151.
5. Hinz, T. 1989. Airborne pollutants from agricultural plants and buildings. In Dodd and Grace (ed.) Agricultural Engineering. Balkema, Rotterdam.
6. Huebner, K. H., and E. Thornton. 1982. The finite element method for engineers. John Wiley & Sons, New York, NY.
7. Leonard, J. J., J. J. R. Feddes, and J. B. McQuitty. 1984. Air quality in commercial broiler housing. Canadian Agric. Engng 26 (1): 65-71.
8. Liao, C. M., and J. J. R. Feddes. 1991. Modeling and analysis of airborne dust removal from a ventilated airspace. Cana-

dian Agric. Engng. 33 (2): 355-361.

9. Liao, C. M. 1992a. Contaminant dispersal analysis in agromicroclimates via lump grouping I. Macroscopic approach. J. Chinese Agric. Engng. 38 (1): 54-68.
10. Liao, C. M. 1992b. Bacteria additives to the change in gaseous mass transfer of swine manure and gas emission rate determination. J. I-Lan Institute of Agric. and Tech. 4: 43-66.
11. Moore, J. W., and R. G. Pearson. 1981. Kinetics and mechanism. John Wiley & Sons, New York, NY.
12. Nauman, E. B., and B. A. Buffham. 1983. Mixing in continuous flow systems. John Wiley & Sons, New York, NY.
13. Wen, C. Y., and L. T. Fan. 1975. Models for flow systems and chemical reactors. Dekker, New York.

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