由團塊群法研析農業微氣候之污染質散佈(一)巨觀法

Contaminant Dispersal Analysis in Agromicroclimates Via Lump Grouping (I) Macroscopic Approach

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摘　要

根據農業微氣候氣流系統可理想化爲一氣流團塊連接離散系統節點之集合群之觀念可推導出一污染質散佈分析模式。系統節點可視爲農業設施及其空氣輸送系統之完全混合空間。統禦農業微氣候中氣流程序及考慮污染質產生或去除之散佈方程式可藉由每個團塊空間質量守恆之基本要求群集團塊方程式而得。本文詳論最後所導得之系統方程式其特性及其穩定與動態解技巧。對實際問題所涉及之污染質散佈分析例之模式應用亦有論述。

關鍵詞：污染質散佈分析、農業微氣候系統、團塊群法、離散分枝技巧、巨觀法。

ABSTRACT

A contaminant dispersal analysis model is presented based upon the concept of the idealization of an agromicrocilimate airflow system as a grouping of flow lumps connected to discrete system nodes corresponding to well-mixed air zones within the agricultural structure and its air delivering system. Equation governing the airflow processes in the agromicroclimate system and equation governing the contaminant dispersal due to this flow, accounting for contaminant generation or removal, are formulated by grouping lump equation so that the fundamental requirement of conservation of mass is satisfied in each zone. The characteristic and solution of the resulting system equation is discussed and steady and dynamic solution methods outlined. Examples of application of this model to practical problems of contaminant dispersal analysis are also presented.

Keywords: contaminant dispersal analysis, agromicroclimate systems, lump grouping, discrete analysis techniques, macroscopic approach.

INTRODUCTION

Airborne contaminants introduced into or generated from an agromicroclimate system disperse throughout the system in a complex manner that depend on the nature of air movment into (supply), out of (exhaust), and within the system, the influence of heating, ventilating, and air conditioning (HVAC) systems on air movement, the possibility of removal by filtration, or contribution by generation; of contaminants by HVAC system, and the possibility of chemical reaction or physico-chemical reaction (e.g., adsorption or absorption) of contaminants with each other or the materials of the systems construction.

The objective of this paper is to develop a model of this dispersal process for an agromicroclimate system that comprehensively accounts for all of these processes that affect the actual contaminant dispersal phenomena. It shall attempt to develop this modeling capability within a more general context so that techniques developed here may be extended to more complex problems of contaminant dispersal analysis.

The airflow system in an agromicroclimate system may be considered to be a three-dimensional field within which the state of infinitesimal air zones (lumps) are seeked to completely describe. The state of air lump will be defined by its temperature, pressure, velocity, and contaminant concentration (for each species of interest) –– the state variables of the contaminant dispersal modeling problem.

The work is then to determine the spacial and temporal variation of the species concentration within a system due to thermal, flow, and concentration excitation driven by environmental conditions and the air delivering system and its control given system characteristics and their control. That is, the purpose is to determine,

$C^{\alpha}(X, y, z, t),$

$C^{\beta}(x, y, z, t),$

$\ldots,$

where:

C = species mass concentration, kg/kg air,
α, β = contaminant species types indices,
x, y, z = spacial coordinates,
t = time, hr,

and shall refer to the process of determining the spacial and temporal variation of these species concentrations as contaminant dispersal analysis.

Contaminant dispersal analysis, for a single nonreactive species α, depends on the air velocity and its variation with time;

$$C^{\alpha}(x, y, z, t) = C^{\alpha}(\vec{v}(x, y, z, t)) \textit{ and B.C.} \tag{1}$$

where B.C. = boundary conditions. But the air velocity field depends on the pressure field which is affected by the temperature field through buoyancy and, completing the circle, the temperature field is dependent on the velocity field:

$$v(x, y, z, t) = v(P(x, y, z, t)) \,\&\, B.C. \tag{2}$$

$$P(x, y, z, t) = P(T(x, y, z, t)) \,\&\, B.C. \tag{3}$$

$$T(x, y, z, t) = T(v(x, y, z, t)) \,\&\, B.C. \tag{4}$$

Thus, contaminant dispersal analysis, for a single nonreactive species, is complicated by a coupled nonlinear flow-thermal analysis problem. Therefore, a comprehensive dispersal model will eventually have to address the related flow and thermal problem. For cases of reactive contaminants, contaminant dispersal analysis itself will become a coupled (and, generally, nonlinear) analysis problem as individual species' concentration depends on other species' concentration in addition to the air velocity field; i.e.,

$$C^{\alpha}(x, y, z, t) = C^{\alpha}(\vec{v}, C^{\beta}, C^{\gamma}, \ldots) \tag{5a}$$

$$C^{\beta}(x, y, z, t) = C^{\beta}(\vec{v}, C^{\alpha}, C^{\gamma}, \ldots) \tag{5b}$$

In this paper the focus will be on single, nonreactive species dispersal analysis and the associated problem of flow analysis, for a completely defined thermal field and its variation. The approach taken has been formulated to be compatiable with lumped-parameter modeling techniques developed earlier by author (Liao and Feddes, 1990; Liao et al., 1991a and 1991b).

Presently, the second paper are addressing the reactive, multiple species dispersal analysis problem.

MODELING APPROACHES

The general field problem posed above shall be attempted to solve by determining the state of air at discrete points in the argomicroclimate airflow system. It will be shown that this spacial discretization allows the formulation of systems of ordinary differential equation that describe the temporal variation of the state fields. Two basic approaches may be considered, one based upon the microscopic equations of motion (i.e., continuity, motion, and energy equations of fields) and the other based upon a well-mixed airspace simplication of macroscopic mass, momentum, and energy balances for flow systems.

In the microscopic modeling approach one of several techniques of the generalized finite element method, which includes the finite difference method (Zienkievicz and Morgan, 1983), could be used to transform the systems of governing partial differential equations into systems of ordinary differential equations that then can be solved using a variety of numerical method. The macroscopic modeling approach leads directly to similar systems of ordinary differential equations.

In both approaches the agromicroclimate airflow system is modeled as a group of discrete flow lumps connected at discrete system nodes. Systems of ordinary differential equations governing the behavior of lumps are then formed and grouped to generate systems of ordinary differential equations that describe the behavior of the system as a whole (i.e., in terms of the spacial and temporal variation of the discrete state variables). These systems of equations may then be solved – given system excitation, initial conditions, and boundary conditions – to complete the analysis.

From a practical point of view, microscopic modeling will involve on the order of 1000 node nodes per airspace, while the macroscopic model will involve on the order of only 10 nodes per airspace to idealize acceptably accurate results. With six state variables for a single species – temperature, pressure, three velocity components and species concentration – the microscopic modeling approach can lead to extremely large systems of equation that therefore limit its use to research inquiry. The macroscopic approach, resulting in systems of equation that are on the order of two magnitudes smaller than the microscopic approach, is a reasonable methodology for partial approach, althrough it can not provide the detail of the microscopic approach. Within this paper, it shall limit consideration to the macroscopic approach.

The agromicroclimate airflow system shall be modelled as a group of flow lumps connected to discrete system nodes corresponding to well-mixed airspace. Limiting the attention to the contaminant dispersal and associated with each system node, the discrete variables or degrees of freedom (DOFs) (Huebner and Thornton, 1982) of pressure, air mass generation (typical airspace), species concentration, species mass generation, and temperature;

$$\{P\} = \{P_1,\ P_2,\ \ldots\}: \textit{Pressure DOFs} \quad (6)$$

$$\{w\} = \{w_1,\ w_2,\ \ldots\}: \textit{air mass generation DOFs} \quad (7)$$

$$\{C\} = \{C_1,\ C_2,\ \ldots\}: \textit{species concen. DOFs DOFs} \quad (8)$$

$$\{S\} = \{S_1,\ S_2,\ \ldots\}: \textit{species generation DOFs} \quad (9)$$

$$\{T\} = \{T_1,\ T_2,\ \ldots\}: \textit{Temperature DOFs} \quad (10)$$

as well as the key system characteristic of nodal volumetric mass, $V_1, V_2, \ldots$. The pressure, concentration, and temperature DOFs will approximate the corresponding values of the state field variables at the spacial locations of the system nodes. With each lump "e" in the system group, the lump connectivity (the system nodes that the lump connects) can be noted and identified a lump air mass flow rate as, w^e. The lump mass rate will be related to the nodal state variables through specific properties associated with each particular lump to form lump equations.

CONTAMINAANT DISPERSAL ANALYSIS

Lump Equations

Two nodes and a total mass flow rate, w^e, will be associated with each flow lump, where flow from node i to j is defined to be positive. A lump species concentration, C_k^e, and a lump species mass flow rate, w_k^e, with each lump node, k= i, j. The lump species mass flow rate is defined so that flow from each node into the flow lump is positive.

It follows from fundamental consideration that these lump variables are related to the total mass flow rate of flow lump as:

$$\{w^e\} = |w^e| \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} \{C^e\}\text{; for } w^e \geqslant 0 \quad (11a)$$

$$\{w^e\} = |w^e| \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix} \{C^e\}\text{; for } w^e \leqslant 0 \quad (11b)$$

or

$$\{w^e\} = [f^e]\,\{C^e\} \quad (11c)$$

where:

$\{w^e\} = \{w_i^e, w_j^e\}^T$; lump species mass flow rate vector, kg/hr (air exchange/hr),

$\{C^e\} = \{C_i^e, C_j^e\}^T$; lump species concentration vector, kg/kg air,

$[f^e]$ = lump total mass flow rate matrix, kg/hr

$$= |w^e| \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}\text{; for } w^e \geqslant 0 \quad (11d)$$

$$= |w^e| \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix}\text{; for } w^e \leqslant 0 \quad (11e)$$

For the purposes there, lump nodes will be selected to correspond to species nodes, consequently, the lump nodal species concentration will have a one-to-one correspondence with the corresponding system node species concentration.

If the flow lump acts as a filter and removes a fraction, η, of the contaminant passing through the filter, then the lump flow rate matrix becomes:

$$[f^e] = |w^e| \begin{bmatrix} 1 & 0 \\ (\eta\text{-}1) & 0 \end{bmatrix}\text{; for } w^e \geqslant 0 \quad (11f)$$

$$= |w^e| \begin{bmatrix} 0 & (\eta\text{-}1) \\ 0 & 1 \end{bmatrix}\text{; for } w^e \leqslant 0 \quad (11g)$$

The fraction, η, is commonly known as the "filter efficiency" and may have values in the range of 0.0 – 1.0.

System Equations

System equations that relate the system concentration DOFs, $\{C\}$, to the system generation DOFs, $\{S\}$, may be grouped from the lump equation by first transforming the lump equation to the system DOFs and then demanding conservation of species mass flow at each system node.

There exists a one-to-one correspondence between each lump's concentration DOFs, $\{C^e\}$, and the system concentration DOFs, $\{C\}$, that may be defined by a simple Boolean transformation;

$$\{C^e\} = [B^e]\,\{C\} \quad (12)$$

where $[B^e]$ is an mxn Boolean transformation matrix consisting zeros and ones; m = the number of lump nodes (here, m=2); n = the number of system nodes.

For example, a lump with nodes i and j (or 1 and 2) connected to the system nodes 5 and 9, respectively, of a 12-node system would have ones in the 1st row, 5th column and the 2nd row, 9th column and all other lumps of the 2x12 Boolean transformation matrix would set equal to zero.

In a similar manner, a system-sized vector can be defined to represent the net species mass flow rate from the system node into a flow lump "e", $\{W^e\}$, and relate to the corresponding lump species mass flow rate using the same transformation matrix as;

$$\{W^e\} = [B^e]^T\{w^e\} \quad (13)$$

For an arbitrary system node n, with connected lump "a", "b", . . . , conservation of species mass then can be shown as;

{(sum of lump species mass flow)
+ (rate of change of species mass)
= (generation of species mass)} node n (14)

or

$$w_n^a + w_n^b + \ldots + V_n dC_n/dt = S_n \tag{15}$$

or for the system as a whole;

$$\sum_{e=a,b,\ldots,} \{W^e\} + [V]\{dC/dt\} = \{S\} \tag{16}$$

where:

[V] = diag ($V_1, V_2, \ldots$); the system volumetric mass matrix, kg,
V_i = the volumetric mass of node i, kg.

Substituting relations (11c), (11c), (12), and (13) into (16) leads to:

$$[F]\{C\} + [V]\{dC/dt\} = \{S\} \tag{17a}$$

where:

$$[F] = \sum_{e=a,b,\ldots} [B^e]^T [f^e] [B^e] \tag{17b}$$

[G] = the system mass flow matrix, kg/kg air,
= G($[f^e]$); the direct grouping sum of lump flow matrix.

Equation (17a) defines the contaminant dispersal behavior of the system as a whole and is said to be grouped from the lump equation through the relation given by equation (17b). The grouping process, as formally represented in equation (17b) is governed by conservation principles. Therefore, G(•) in equation (17b) can be referred to as the grouping operator.

Boundary Conditions

The variation of concentration or generation rate, but not both, may be specified at system nodes. Concentration or generation conditions in the discrete model are equivalent to boundary conditions in the corresponding continuum model.

Formally, these DOFs for which concentration will be specified, $\{C_c\}$, may be distinguished from those for which generation rate be specified, $\{C_s\}$, and partition the system of equations accordingly;

$$\begin{bmatrix} [F_{cc}] & [F_{cs}] \\ [F_{sc}] & [F_{ss}] \end{bmatrix} \begin{Bmatrix} \{C_c\} \\ \{C_s\} \end{Bmatrix} + \begin{bmatrix} [V_{cc}] & [0] \\ [0] & [V_{ss}] \end{bmatrix} \begin{Bmatrix} \{dC_c/dt\} \\ \{dC_s/dt\} \end{Bmatrix} = \begin{Bmatrix} \{S_c\} \\ \{S_s\} \end{Bmatrix} \tag{18}$$

using the second equation and simplifying, it leads to;

$$[F_{ss}]\{C_s\} + [V_{ss}]\{dC_s/dt\} = \{S_s\} - [F_{sc}]\{C_c\} \tag{19b}$$

or

$$[\hat{F}]\{\hat{C}\} + [\hat{V}]\{d\hat{C}/dt\} = \{\hat{E}\} \tag{19b}$$

where:

$[\hat{F}] = [F_{ss}]$ = the generation driven mass flow matrix,
$\{\hat{C}\} = \{C_s\}$ = the generation driven nodal concentration,
$\{\hat{E}\} = \{S_s\} - [F_{sc}]\{C_c\}$ = the system excitation.

It should be noted that the response of the system is driven by the system exictation involving both species concentration mass generation rates and contaminant concentration which may vary with time.

Equation (19b) written in the standard form of a set of first ordinary differential equation similar to the form of equation (17a), directly defines the contaminant dispersal behavior of the system. The formation and solution of equation (19b) will be considered as a central task of contaminant dispersal analysis.

The response of the system is defined by the solution of equation (19b) for the generation rate specified DOFs, $[C_s]$. The generation rates, $\{S_c\}$, required to maintain the specified concentration $\{C_c\}$, may be determined from the repsonse of the system to the specified excitation excitation using the first equation of equation (18), as:

$$\{S_c\} = [F_{cc}]\{C_c\} + [F_{cs}]\{C_s\} + [V_{cc}]\{dC_c/dt\} \tag{20}$$

Qualitative Analysis of System Equation

System flow matrix

The system flow matrix [F], being a direct grouping sum of nonsymmetric lump matrices, will also be nonsymmetric. The details of the grouping process reveal that the diagonal elements of the flow matrix are always positive and the off-diagonal elements negative. Furthermore, if the total mass flow rate into a system node is equal to the total mass flow rate out of a system node, then the diagonal elements of the flow matrix will be less than or equal to the row sum or the column sum of the corresponding off-diagonal element, F_{ii}, is simply equal to the total mass flow rate out of a node, the row sum of row i equals to the sum of total mass flow rate into the node weighted by the filter efficiency factor ($\eta - 1$);

$$\textit{row sum of row } i \equiv \sum_{\substack{j=1 \\ j\neq i}}^{n} |F_{ij}| \tag{21}$$

and the column sum equals to the sum of total mass flow out of the node weighted by the filter efficiency factor ($\eta - 1$);

$$\textit{column sum of col. } i \equiv \sum_{\substack{j=1 \\ i\neq j}}^{n} |F_{ji}| \tag{22}$$

Therefore, if total mass flow is conserved at each node, it can be asserted that,

$$F_{ii} \geqslant \sum_{\substack{j=1 \\ j\neq i}}^{n} |F_{ij}| \tag{23}$$

and,

$$F_{ii} \geqslant \sum_{\substack{j=1 \\ i\neq j}}^{n} |F_{ji}| \tag{24}$$

where the equality is strict when filter efficiencies of the lumps connected to node i are zero (i.e., all η=0) and the inequality holds if any of the connected outflow lumps (for the row sum) or inflow lumps (for the column sum) have nonzero filter efficiencies.

If all lumps of a flow system idealization have nonzero filter efficiencies then the system flow matrix will be strictly diagonally dominant; a condition that can prove the flow matrix would be nonsingular. For the unlikely limiting case where all lumps have filter efficiencies equal to 1.0, the flow matrix becomes diagonal and, therefore, all zeros act as independent (i.e., uncoupled) single zone system.

If all lumps have filter efficiencies equal to 0.0, the equality of equations (23) and (24) hold for all nodes and the flow matrix is no longer strictly diagonally dominant, and therefore, may not be assumed to be nonsingular. It can be shown that the important submatrix of the flow matrix is nonsingular be demanding conservation of total mass flow of all subgrouping of system nodes and their inter-connecting lumps and using some theorems relating to the general class of matrices known as M-matrices.

A M-matrix is a square nonzero real matrix with all off-diagonal elements nonpositive that has eigenvalues with nonnegative real parts (Funderlic and Plemmons, 1981). It may be shown (Plemmons, 1979) that a real square matrix [A], with positive diagonal elements and nonpositive off-diagonal elements; (i) is an M-matrix if and only if it can be shown that [[A] + ξ[I]] is a nonsingular M-matrix for all scaler $\xi >$ 0, and (ii) is a nonsingular M-matrix if [A] is strictly diagonally dominant.

As can be seen that [[F] + ξ[I]] is strictly diagonally dominant, and therefore a nonsingular M-matrix, for all scalar $\xi > 0$. Thus, it can be concluded that [F] is an M-matrix, althrough it will be singular for the limiting case when all filter efficiencies are zero.

It has also been shown that each principal submatrix of an irreducible M-matrix is a nonsingular M-matrix (Plemmons, 1979). The flow matrix would be said to be reducible if it is possible, using an appropriate numbering of the system nodes, to group the flow matrix in the permuted form,

$$[F] = \left[\begin{array}{cc} [F_{11}] & [F_{12}] \\ \hline [0] & [F_{22}] \end{array}\right] \quad (25)$$

where $[F_{11}]$ and $[F_{22}]$ are square matrices, otherwise [F] would be said to irreducible. Recalling that superdiagonal term, F_{ij}; $j > i$, corresponds to flow from node j to node i and a subdiagonal term, F_{ji}, $j > i$, corresponds to flow from node i to node j, a flow matrix of the form of equation (25) would correspond to a flow system idealization having a total mass flow subgrouping 2 to subgrouping 1, without a return flow from 1 to 2, and therefore, conservation of total mass flow would be violated.

It may be conclluded that; (i) the flow matrix [F] will be an irreducible M-matrix, and therefore (ii) the generation driven mass flow matrix, $[\hat{F}]$, a principal submatrix of the flow matrix will be a nonsingular M-matrix, if they are found based upon a flow idealization that satisfies conservation of total mass flow.

Thus the solution of the generation driven contaminant dispersal equation (equation (19b)) is the central task of contaminant dispersal analysis, and the nonsinguality of the generation driven flow matrix is a necessary condition to assume the possibility of solution of these equations.

System volumetric mass matrix

By definition the system volumetric mass matrix, [V], is diagonal and nonsingular. When some nodal volumetric masses are so smallthat the analyst prefers to model them with zero values, the system of contaminant dispersal equations may be reduced (by eliminating the massless equations) to a form having an all positive. Thus, a nonsingular volumetric mass matrix is obtained. The inverse of the positive volumetric mass matrix then becomes,

$$[V]^{-1} = diag\,[1/V_1, 1/V_2, \ldots, 1/V_n]; \quad V_i \neq 0 \quad (26)$$

System equation – steady flow

The generation driven contaminant dispersal equation (equation (19b)) may be written in the form as:

$$[\hat{V}]^{-1}[\hat{F}]\{\hat{C}\} + \{d\hat{C}/dt\} = [\hat{V}]^{-1}[\hat{E}] \quad (27)$$

where the $[\hat{F}]$ will be varied with time.

The product matrix $[\hat{V}]^{-1}[\hat{F}]$ contains the essential dynamic characteristics of the system being studied. For properly formed idealizations (being the product of a positive diagonal matrix and a nonsingular M-matrix (Graybill, 1983)) it will be a nonsingular M-matrix, and therefore solution to equation (27) will exist.

It can be gained some insight into the general character of solution to equation (27) by considering the case of steady flow ($[\hat{F}]$ constant) without excitation (i.e., the homogeneous case);

$$[\hat{V}]^{-1}[\hat{F}]\{\hat{C}\} + \{dC/dt\} = \{0\} \quad (28)$$

the solution to equation (28) will be as follows;

$$\{C\} = \{\Phi\}\,exp(-t/\tau) \quad (29)$$

where:

τ = decay time constant,
$\{\Phi\}$ = vector of unknown magnitudes.

Substituting equation (29) into equation (28) leads to the standard eigenvalue problem,

$$[[\hat{V}]^{-1}[\hat{F}] - (1/\tau)[I]]\{\Phi\} = \{0\} \quad (30)$$

the solution of this standard eigenvlaue problem and its relation to the first order system of differential being considered is discussed elsewhere (Noble and Daniel, 1988; Strang, 1980). For a properly formed flow system idealization of n nodes there will be n solution to this eigenvalue problem consisting of n pairs of time constants, ι (or equivalently their inverse, $1/\tau$ – the system eigenvalues) and their associated eigenvcetors, $\{\Phi\}$.

In some case it may be possible to transform the product matrix $[\hat{V}]^{-1}[\hat{F}]$, by similarity transformation, to diagonal form leaving the eigenvalues on the diagonal as:

$$[T]^{-1}[[\hat{V}]^{-1}[\hat{F}][T] = diag\,[1/\tau_1, 1/\tau_2, \ldots, 1/\tau_n] \quad (31)$$

where [T] is the similarity transformation.

For these cases it will be possible to express the general solution to the homogeneous problem, equation (28), as a linear combination of simple exponential decay terms:

$$\{C(t)\} = a_1\{\Phi\}exp(-t/\iota_1) + a_2\{\Phi\}exp(-t/\iota_2) + ... + a_n\{\Phi_n\}\, exp(-t/\tau_n) \quad (32)$$

where the scalar coefficients, $a_1, a_2, \ldots, a_n$ are determined from the initial conditions using similarity transformation employed as:

$$\{a\} = [T]^{-1}\{C(0)\} \quad (33)$$

The n pairs of time constants and asociated eigenvectors are often referred to as the eigenmodes of the system (Palm, 1983) and the response of the system is often described in terms of the degree to which each eigenmode participates. From the form of the free response (equation (32)), it is clear that as time passes the contribution of those eigenmodes with larger time constants will dominant the character of the response until the response in all zones will be dominated by the eigenmode with largest time constant and therefore will appear to be a simple exponential decay.

For general contaminant dispersal systems the Gerschgorin circles (Noble and Daniel, 1988) may be applied, given the volumetric mass matrix is diagonal, to obtain a poorly bounded, but computationally inexpensive, estimate of the real part of system time constants as;

$$1/t \leqslant 1/V_i(\hat{F}_{ii} \pm \sum_{j=1,2,...}^{j\neq i} \hat{F}_{ij}), \mathit{for\ all\ i.} \quad (34)$$

When all filter efficiencies are 0.0, it assumes only that the system time constant will fall within the range (Noble and Daniel, 1988);

$$Min(V_i/(2\hat{F}_{ii})) \leqslant \iota \leqslant \infty, \mathit{all}\ \eta_s = 0.0 \quad (35)$$

as, in these cases the off-diagonal row sum will be equal to the diagonal values of the flow matrix.

In all cases the system time constants will have positive real parts, as the product matrix is a nonsingular M-matrix, and therefore all components making up the general solution will approach zero with time. That is to say, the homogeneous contaminant dispersal equations are stable, the concentrations at all nodes will approach zero. Furthermore, it can be seen that the sum of the product matrix and its transpose,

$$[[\hat{V}]^{-1}[\hat{F}] + [[\hat{V}]^{-1}[\hat{F}]]^T]$$

is also a nonsingular M-matrix with positive real part of eigenvalues and, therefore, the sum of the squares of system concentrations (i.e., the (Euclidean norm of the concentration vector) will decay at very instant of time (Strang, 1980):

$$d\|\{C(t)\}\|^2/dt < 0,\ t \geqslant 0 \quad (36)$$

where:

$$\|\{C(t)\}\|^2 \equiv (|C_1(t)|^2 + |C_2(t)|^2 + ... + |C_n(t)|^2).$$

The response of steady flow systems to nonzero excitation (i.e., nonhomogeneous case) may also be expressed in terms of linear combination of the eigenvectors of the product matrix $[\hat{V}]^{-1}[\hat{F}]$. For practical contaminant dispersal analysis, it is more convenient to solve the system equation directly using numerical integrants techniques that are not limited to steady flow cases.

Solution of System Equations

Steady state behavior

For systems with steady lump mass flow driven by steady contaminant generation rates and/or specificed concentrations the response of the system will, eventually, come to a steady state (i.e., $\{d\hat{C}/dt\} = 0$) given by the solution of,

$$[\hat{F}]\{\hat{C}\} = \{\hat{E}\} \quad (37)$$

Free response behavior

The free response behavior of steady flow system has been discussed above and shown to be closely related to the solution of the eigenproblem given by equatinon (30) that yields system time constants and associated eigenvectors.

For steady flow system knowledge of the system time constants provides invaluable insight into the dynamic character of the system yet eigenanalysis is computationally time consuming. Thus, it is attempting to estimate the system time constants, after single-zone theory, by the ratio of the volumetric mass of each zone to the total air flow out of the zone. This estimate of system time constants will be designed as the nominal system time constants and, may be represented as,

$$\tau_i \equiv V_i/F_{ii} \tag{38}$$

For typical situations, the error bound on this estimate is very large and this estimate of the actual system time constants is likely to be a very poor estimate. A variety of techniques exist that will provide better solution to governing eigenvalue problem and thereby provide better estimates of the actual system time constants (Wilkinson and Reinsch, 1971).

Dynamic behavior

The governing systems of equation (equation (19b)) may be solved for cases of steady flow with general unsteady contaminnat generation rates using any number of different finite difference solution schemes. Here a general form predictor-corrector method will be employed or referred to as generalized trapezoid rule.

For cases of unsteady flow it is likely that this same predictor-corrector solution scheme will prove useful, if the system flow matrix, $[F]$, is updated appropriately, although for cases of rapidly changing flow rates small time steps may be required to control errors. If difficulties arrive, an interactive scheme may have to be nested within the predictor-corrector time integration scheme.

A finite difference scheme for the approximate integration of the semidiscrete equation (19b) may be developed by dividing time domain into discrete steps,

$$t_{(n+1)} = t_{(n)} + \delta t,\ n = 0,\ 1, \ldots,\ (n+2) \tag{39}$$

where:

$t_{(0)}$ = initial time,
δt = integration time step.

Demanding the satisfaction of equation (19b) at each of these steps (Huebner and Thornton, 1982),

$$[\hat{F}]\{\hat{C}\}_{(n+1)} + [\hat{V}]\{d\hat{C}/dt\}_{(n+1)} = \{\hat{E}\}_{(n+1)} \tag{40}$$

where:

$$\{\hat{C}\}_{(n+1)} \equiv \{\hat{C}(t_{(n+1)})\},$$

$$\{d\hat{C}/dt\}_{(n+1)} \equiv \{d\hat{C}(t_{(n+1)})/dt\},$$

$$\{\hat{E}\}_{(n+1)} \equiv \{\hat{E}(t_{(n+1)})\}.$$

Substituting into these equation, the consistent difference approximation represented by;

$$\{\hat{C}\}_{(n+1)} \cong \{\hat{C}\}_{(n)} + (1-\theta)\delta t\{d\hat{C}/dt\}_{(n)} + \theta\delta t\{d\hat{C}/dt\}_{(n+1)},\ 0 \leqslant \theta \leqslant 1, \tag{41}$$

where $\theta = 0$ corresponds to the Forward Difference scheme, $\theta = 1/2$ corresponds to Crank-Nicholson scheme, $\theta = 2/3$ corresponds to Galerkin scheme, and $\theta = 1$ corresponds to Backward Difference scheme.

A general implicit finite difference scheme is formulated (Huebner and Thornton, 1982):

$$[\theta\delta t[\hat{F}] + [\hat{V}]]\{d\hat{C}/dt\}_{(n+1)} \cong \{\hat{E}\}_{(n+1)} - [\hat{F}](\{\hat{C}\}_{(n)} + (1-\theta)\delta t\{d\hat{C}/dt\}_{(n)}) \tag{42a}$$

or, equivalently;

$$[[\hat{F}] + (1/(\theta\delta t)[\hat{V}]]\{\hat{C}\}_{(n+1)} \cong [\hat{E}]_{(n+1)} + 1/(\theta\delta t)[\hat{V}]\{\hat{C}\}_{(n)} + (1-\theta)\delta t\{d\hat{C}/dt\}_{(n)} \tag{42b}$$

Computationally it is useful to implement this general finite difference scheme (equation (42)) as a three steps predictor-corrector algorithm;

(1) $\{\tilde{C}\}_{(n+1)} \equiv \{\hat{C}\}_{(n)} + (1-\theta)\delta t\{d\hat{C}/dt\}_{(n)}$, *predictor* (43a)

(2) $[(\theta\delta t)[\hat{F}¼ + [\hat{V}]]\{d\hat{C}/dt\}_{(n+1)} \cong \{\hat{E}\}_{(n+1)} - [\hat{F}]\{\tilde{C}\}_{(n+1)}$ (43b)

(3) $\{\tilde{C}\}_{(n+1)} \cong \{\tilde{C}\}_{(n+1)} + (\theta\delta t)\{d\hat{C}/dt\}_{(n+1)}$, *Corrector* (43c)

This predictor-corrector scheme has been analyzed by Huebner and Thornton (1982) and a more general predictor-multicorrector scheme that includes this implict scheme has been analyzed by Hughens (1985) for systems with constant coefficient matrices (i.e., $[\hat{F}]$ and $[\hat{V}]$ are constants).

MODEL EXAMPLES

Single Zone Examples

It is useful to first consider a single zone airflow system that exchanges indoor air with the exterior environment. Such a single zone system may be modeled as a grouping of two flow lumps, corresponding to inlet and exhaust flow paths, connected to two system nodes, corresponding to the inside air zone and the exterior environment zone as illustrated in Figure 1.

The equations governing this simplest flow system have the following general form;

$$\begin{bmatrix} w_1 & -w_2 \\ -w_1 & w_2 \end{bmatrix} \begin{Bmatrix} C_1 \\ C \end{Bmatrix} + \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix} \begin{Bmatrix} dC_1/dt \\ dC_2/dt \end{Bmatrix} = \begin{Bmatrix} S_1 \\ S_2 \end{Bmatrix} \qquad (44)$$

From a consideration of mass containuity, $w_1 = w_2$ is required and therefore equation (44) may be rewritten in expanded form as:

$$wC_1 - wC_2 + V_1 dC_1/dt = S_1 \qquad (45a)$$

$$-wC_1 + wC_2 + V_2 dC_2/dt = S_2 \qquad (45b)$$

With these equations in hand two cases shall be proceeded to consider: Case 1: Contaminant decay under steady flow condition, and Case 2: Contaminant decay under unsteady flow condition.

Case 1: Consider the particularly simple, and familiar case of contaminant decay from some initial value, $C_1(t = 0)$, under steady flow conditions (w = constant) with concentration in the exterior environment maintained at the zero level, $C_2 = 0$. Under these conditions, equation (45) may be simplified to:

$$wC_1 + V_1 dC_1/dt = 0 \qquad (46)$$

whose exact solution is:

$$C_1(t) = C_1(t{=}0)\exp(-t/(V_1/w)) \qquad (47)$$

where V_1/w = time constant of the system.

The exact solution is compared (Figure 2) to approximate solutions generated using integration time steps of Δt = 2.0, 1.0, and 0.5 hrs with $C_1(t = 0) = 1.0\times10^{-6}$ kg/kg air, V_1 = 31.87 kg (assumed air density of 1.1803 kg/m^3 corresponding to 26°C and 1 atm), w = 12.75 kg/hr (i.e., 0.4 air exchange per hr), and time constant = V_1/w = 2.5 hr.

The accuracy of the general predictor-cor-

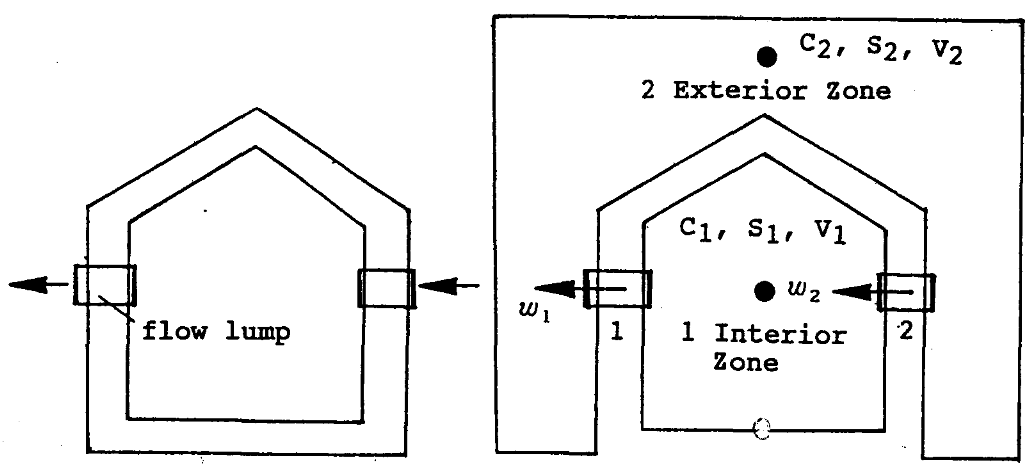

Figure 1. A single zone farm structure and corresponding flow model.

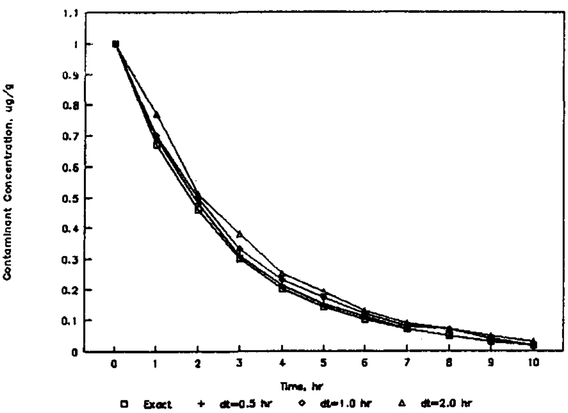

Fig. 2. Single zone model: contaminant decay under steady flow conditions.

rector method used to approximate the response of this system is related to the time constant of the system being studied. In this case the time constant is 2.5 hr. From the results of this single study, it appears that using an integration time increment equal to a fraction of the system time constant will assure practically accurate results.

Case 2: To investigate the consequence of unsteady flow on the nature of the behavior of the real system and the numerical characteristics of its simulation, Case 1 shall be extended by considering the decay of a contaminant under conditions of linearly increasing flow rates, that is to say with;

$$w = w^0 t;\ t \geqslant 0 \tag{48}$$

The decay problem is now governed by the equation

$$w^0 t C_1 + V_1 dC_1/dt = 0,\ C_1(t=0) = 1.0 \tag{49a}$$

or

$$w^0 t dt = -V_1 dC_1/C_1,\ C_1(t=0) = 1.0 \tag{49b}$$

The second from, with variables t and C_1 separated, may be integrated directly to obtain the exact solution,

$$C_1 = 1.0 \exp(-t^2/(2V_1/w^0)) \tag{50}$$

Again this exact solution is compared to approximate solutions (Figure 3).

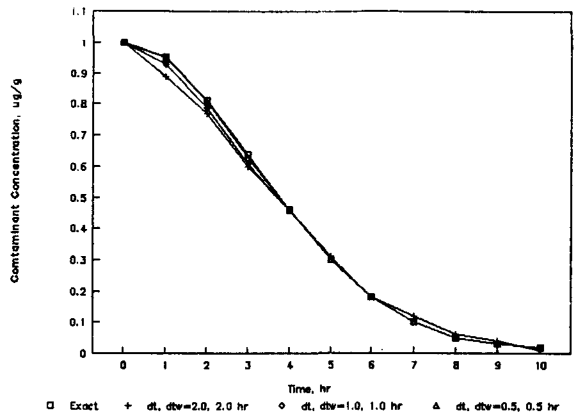

Fig. 3. Single zone contaminant decay under unsteady flow conditions with flow updating at each integration time step.

For this case, the numerical consequence of both integration time step, Δt, and step-wise approximation of the unsteady flow, Δtw, (i.e., the flow approximation time setep) can be considered. (The solution was generated for V_1 = 31.87 kg, and w^0 = 3.187 kg/hr.) In this case, using an integration time step equal to the flow approximation time step, $\Delta t = \Delta tw$, (i.e., updating the system flow matrix at each time step) provides practically accurate results for even the relatively large time step for 2.0 hrs (Figure 3). Updating the system flow matrix every other time step introduces an offset error equal to the flow approximation time step (when compared to results obtained with updating at each time step) for the first time step that is gradually diminished with each successive time step (Figure 4). This initial offset error is caused by the initial zero flow condition.

Contaminant Dispersal Analysis of an Experimental Test

In this case, system characteristics will be based on those of an experimental test reported by Brannigan and McQuitty (1971) involving measurements of contaminants emission from gas diffusion units. The study was carried out in an environmental chamber which dimensions were such as to simulate one pan of a piggery.

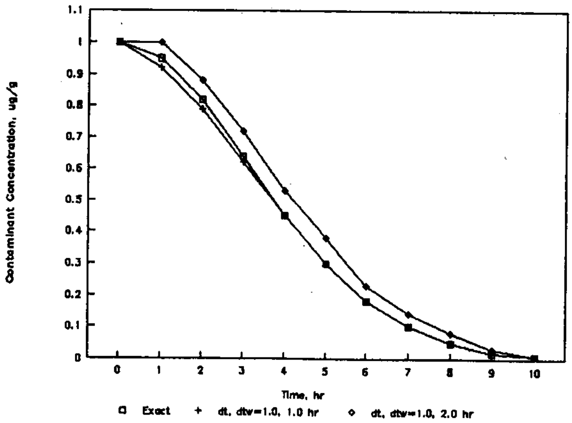

Fig. 4. Single zone contaminant decay under unsteady flow conditions with flow updating at every integration time step.

Estimated capacity of a pan of this size is 20 pigs, each weighting approximately 55 kg. The properties of the system and excitation used in the experimental test are: (1) ventilation rate: 280, 443, and 932 m^3/hr. (2) Contaiminant emission rate: CO_2 = 942 g/hr, NH_3 = 20.4 g/hr (based on CO_2 and NH_3 density of 1.773 and 0.6894 kg/m^3, respectively, corresponding to 26°C and 1 atm).

Brannigan and McQuitty (1971) discussed two kinds of ventilation systems: (1) short-circuiting, and (2) displacement systems. In this case, the environmental chamber can be modeled as a 25-node multi-zone system to study the variations of contaminant concentration generated by gas diffusion units (Figure 5). The airflow patterns of the two ventilation system are schematically shown in Figure 6.

The input data for the contaminant dispersal analysis shall be included: (1) Entrainment ratio, r: in order to determine recirculation flow rate, rw, some estimations of the entrainment ratio, r, is possible on the basic of a simple entrainment concept (Liao and Feddes, 1991; Liao et al., 1991b). Therefore, rw is entirely induced by the primary flow rate, i.e., by the entrainment in the inlet jets, is assumed. For long slot, the entrainment ratio can be determined by (ASHRAE, 1985), r = rw/w = entrainment flow / initial flow = $((2/K')(X/H_0))^{1/2}$, where X

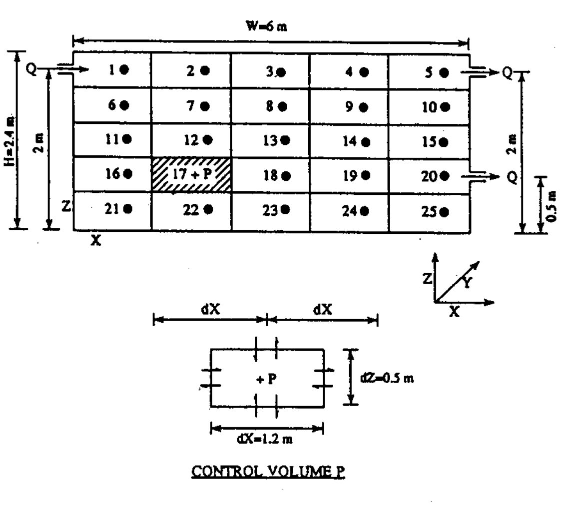

Fig. 5. An environmental chamber modeled as a 25-node multi-zone system.

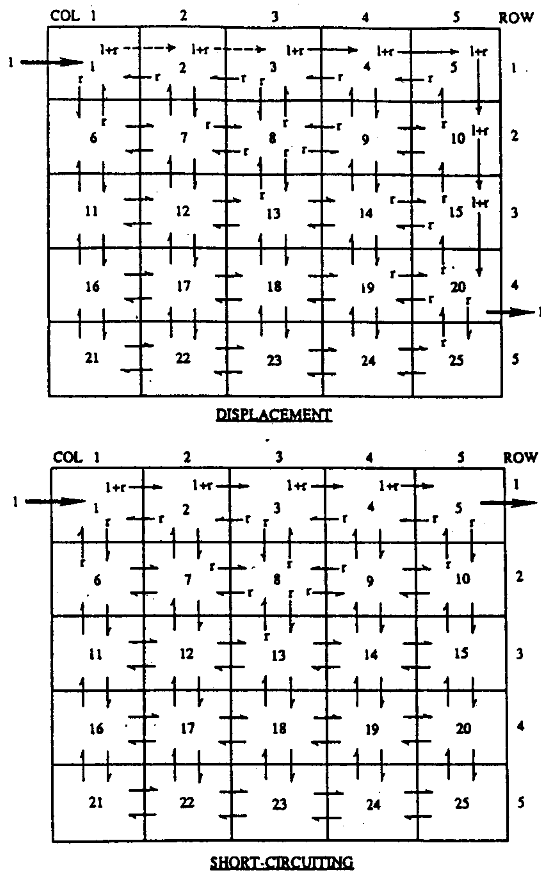

Fig. 6. The air flow patterns for two ventilation systems in simulation model in the case of Brannigan and McQuitty, (1971).

Table 1. Calculated mean equilibrium concentration of NH_3 and CO_2 for two ventilation systems

Ventilation system	Equilibrium contaminant concentration NH_3 (ppm)	CO_2 (ppm)
Displacement	58 (50)[a]	1037 (920)
Short-circuiting	62 (54)	1104 (980)

[a]The number in the parentheses is the measured values reported by Brannigan and McQuitty (1971).

= distance from of outlet (= 6m), H_0 = width of slot (= 51mm), and K′ = proportionality constant (approximately 7). Thus, r = 5.8. (2) System flow matrix $[F]$: the system flow matrix being a direct grouping sum of the solution of lump flow matrices by 2-D lumped form of control volumes represented the conservation of air mass. (3) Volumetric mass matrix $[V]$: each nodal volumetric air mass assumed to be equal. Therefore, V_i = 1.7 kg, i = 1, 2, . . . , 25, based on the reported volume of $36 m^3$ and an air density of 1.1803 kg/m^3 corresponding to 26°C and 1 atm.

The calculated mean equilibrium concentrations of NH_3 and CO_2 at both ventilation systems are listed in Table 1. To convert from units of g/m^3 to ppm (volume), it is assumed that the ideal gas law is accurated under ambient condition (26°C, 1 atm), therefore, the conversion factors for NH_3 and CO_2 form g/m^3 to ppm are 1440 and 560, respectively. Table 1 shows that the simulated results are compared very closed to the measured values.

The mean equilibrium concentration of NH_3 and CO_2 at different ventilation rates changing with height-from-floor and distance-from-inlet are illustrated in Figures 7-10. Figures 7-10 show that at higher ventilation rates the predicted and measured velues are compared very consistent, while a clear discrepancy was observed at low ventilation rates. The reason may be that the assumption of macroscopic complete-mixing used in deriving the system equation does not hold as well for the low airfow rate since the density difference between contaminants and air.

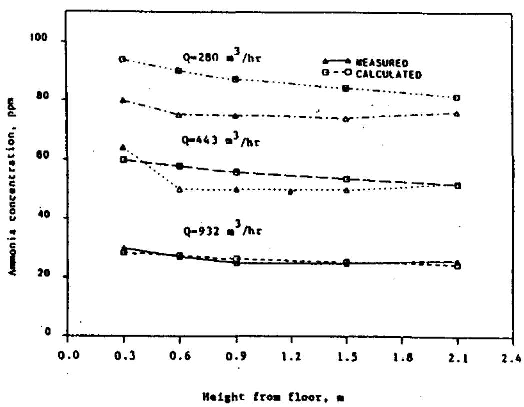

Fig. 7. The comparison of model predicted of ammonia interacted with height-from-floor a and different ventilation rates with that measured by Brannigan and McQuitty (1971).

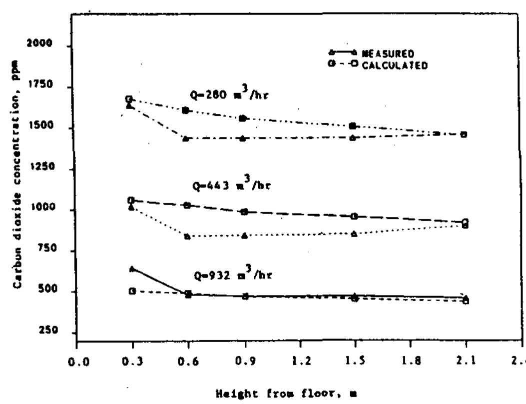

Fig. 8. The comparison of model predicted of carbon dioxide interacted with height-from-floor and different ventilation rates with that measured by Bannigan and McQuitty (1971).

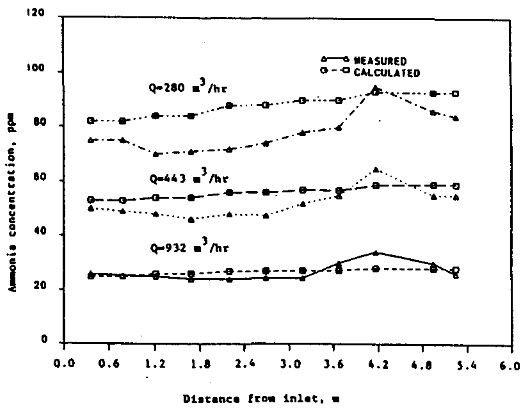

Fig. 9. The comparison of model predicted of ammonia interacted with distance-from-inlet and different ventilation rates with that measured by Brannigan and McQuitty (1971).

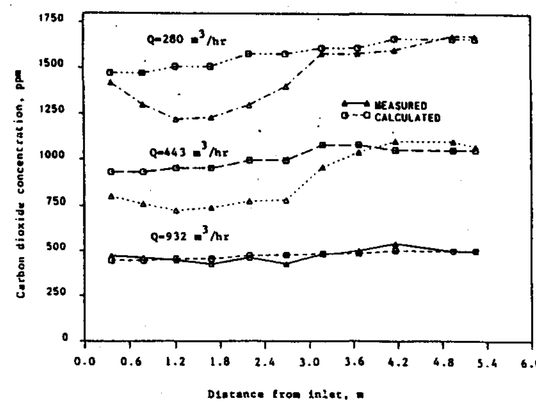

Fig. 10. The comparison of model predicted of carbon dioxide interacted with distance-from-inlet and fiferent ventilation rates with that measured by Brannigan and McQuitty (1971).

Therefore, a significant departure from homogeneity might be expected.

CONCLUSION

1. From a practical point of view, the lump grouping via macroscopic approach is intuitively satisfying and allows consideration of agromicroclimate systems of arbitrary complexity.

2. From a theoretical point of view, it provides a framework for the consideration of the large variety of mass transport processes that affect the contaminant dispersal in farm structures and offers additional mathematical tools to unravel the formal characteristics of whole structure dispersal models.

3. From a research and development point of view, it separates the general problems of contaminant dispersal analysis into two primary subproblems; lump development and development of solution methods. Research efforts can thus be focused on the modeling of specific transport processes, to develop improved or new lumps (e.g., the kinetic and 1-D diffusion-convection lumps) or, alternatively, be focused on developing improved methods for solving the resulting equations while accounting for the complex coupling that may exist between the related thermal, dispersal, and flow analysis problems.

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