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Standard Guide for Simulation of Subsurface Airflow Using Ground-Water Flow Modeling Codes[1]

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1. Scope

1.1 This guide covers the use of a ground-water flow modeling code to simulate the movement of air in the subsurface. This approximation is possible because the form of the ground-water flow equations are similar in form to airflow equations. Approximate methods are presented that allow the variables in the airflow equations to be replaced with equivalent terms in the ground-water flow equations. The model output is then transformed back to airflow terms.

1.2 This guide illustrates the major steps to take in developing an airflow model using an existing ground-water flow modeling code. This guide does not recommend the use of a particular model code. Most ground-water flow modeling codes can be utilized, because the techniques described in this guide require modification to model input and not to the code.

1.3 This guide is not intended to be all inclusive. Other similar techniques may be applicable to airflow modeling, as well as more complex variably saturated ground-water flow modeling codes. This guide does not preclude the use of other techniques, but presents techniques that can be easily applied using existing ground-water flow modeling codes.

1.4 This guide is one of a series of standards on ground-water model applications, including Guides D 5447 and D 5490. This guide should be used in conjunction with Guide D 5447. Other standards have been prepared on environmental modeling, such as Practice E 978.

1.5 The values stated in SI units are to be regarded as the standard.

1.6 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

1.7 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 653 Terminology Relating to Soil, Rock, and Contained Fluids[2]

D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem[3]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[3]

E 978 Practice for Evaluating Environmental Fate Models of Chemicals[4]

3. Terminology

3.1 *Definitions:*

3.1.1 *boundary condition*—a mathematical expression of a state of the physical system that constrains the equations of the mathematical model.

3.1.2 *computer code (computer program)*—the assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output.

3.1.3 *ground-water flow model*—application of a mathematical model to represent a site-specific ground-water flow system.

3.1.4 *mathematical model*—(*a*) mathematical equations expressing the physical system and including simplifying assumptions, (*b*) the representation of a physical system by mathematical expressions from which the behavior of the system can be deduced with known accuracy.

3.1.5 *model*—an assembly of concepts in the form of mathematical equations that portray understanding of a natural phenomenon.

3.2 For definitions of other terms used in this guide, see Terminology D 653.

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[2] *Annual Book of ASTM Standards*, Vol 04.08.

[3] *Annual Book of ASTM Standards*, Vol 04.09.

[4] *Annual Book of ASTM Standards*, Vol 11.04.

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3.3 *Symbols:Symbols and Dimensions:*

3.3.1 A—cross-sectional area of cell [cm ^{2}].

3.3.2 g—acceleration due to gravity [cm/s ^{2}].

3.3.3 h—air-phase or water phase head [cm].

3.3.4 k—air phase permeability [cm^2].

3.3.5 K—hydraulic conductivity [cm/s].

3.3.6 P—air phase pressure [g/cm-s^2].

3.3.7 P_0—reference air-phase pressure [g/cm-s^2].

3.3.8 q_s—specific discharge vector for air [cm/s].

3.3.9 q—volumetric flow of water through cell [cm^3/s].

3.3.10 $q*$—model-computed term related to airflow in units g^2-cm/s^4.

3.3.11 q_v—volumetric airflow [cm ^{3}/s].

3.3.12 q_m—mass airflow [g/s].

3.3.13 R—universal gas constant = 8.314×10^{7}[g-cm^2/s^2-mol-K].

3.3.14 S_s—specific storage of the porous material [cm^{-1}].

3.3.15 t—time [s].

3.3.16 T—temperature [K].

3.3.17 W—volumetric flux per unit volume [s $^{-1}$].

3.3.18 z—elevation head [cm].

3.3.19 ∂h—hydraulic head difference [cm].

3.3.20 ∂l—length of model cell [cm].

3.3.21 ρ—density of air [g/cm ^{3}].

3.3.22 θ—air-filled porosity [nd].

3.3.23 ϕ—pressure-squared (P ^{2}) [(g/cm-s^2)^2].

3.3.24 ω—average molecular weight of air [g/mol].

3.3.25 μ—dynamic viscosity of air [g/cm-s].

4. Summary of Guide

4.1 The flow of gas (air in this case) through unsaturated porous media can be approximated using ground-water flow modeling codes. This is accomplished through substitution of air-phase parameters and variables into the ground-water flow equations. There are two substitution techniques discussed in this guide, the pressure-squared technique **(1)**, and the pressure substitution technique **(2)**. These substitutions are summarized as follows:

4.1.1 The dependent variable, usually head, in the ground-water flow equation becomes pressure or pressure-squared;

4.1.2 Saturated hydraulic conductivity (K), both horizontal and vertical components, becomes air permeability (k or intrinsic permeability) in the pressure-squared technique and an equivalent air hydraulic conductivity in the pressure substitution technique.

4.1.3 Storage coefficient (S) becomes the air storage coefficient (S_a);

4.1.4 The Vadose zone is considered a confined aquifer; and,

4.1.5 All boundary conditions are expressed in terms of air pressure-squared, although constant flux boundary conditions may be used in the pressure substitution technique.

4.2 The ground-water modeling code is executed using these parameter and variable substitutions. The model results must then be transformed to values representative of air. These calculations are summarized as follows:

4.2.1 If the problem is formulated in terms of air pressure-squared, the square root of the model-computed dependent variable is computed at each cell;

4.2.2 Flow rates computed by the pressure-squared approach must be transformed into equivalent airflow terms for volumetric flow rates (q_v) or mass flow rates (q_m).

4.2.3 No transformation of the output is required by the pressure substitution technique, although the pressures may be converted to more convenient units.

5. Significance and Use

5.1 The use of vapor extraction systems (VES), also called soil vapor extraction (SVE) or venting systems, is becoming a common remedial technology applicable to sites contaminated with volatile compounds **(3, 4)**. A vapor extraction system is composed of wells or trenches screened within the vadose zone. Air is extracted from these wells to remove organic compounds that readily partition between solid or liquid phases into the gas phase. The volatile contaminants are removed in the gas phase and treated or discharged to the atmosphere. In many cases, the vapor extraction system also incorporates wells open to the atmosphere that act as air injection wells.

NOTE 1—Few model codes are available that allow simulation of the movement of air, water, and nonaqueous liquids through the subsurface. Those model codes that are available **(5, 6)**, require inordinate compute hardware, are complicated to use, and require collection of field data that may be difficult or expensive to obtain. In the future, as computer capabilities expand, this may not be a significant problem. Today, however, these complex models are not applied routinely to the design of vapor extraction systems.

5.2 This guide presents approximate methods to efficiently simulate the movement of air through the vadose zone. These methods neglect the presence of water and other liquids in the vadose zone; however, these techniques are much easier to apply and require significantly less computer hardware than more robust numerical models.

5.3 This guide should be used by ground-water modelers to approximately simulate the movement of air in the vadose zone.

5.4 Use of this guide to simulate subsurface air movement does not guarantee that the airflow model is valid. This guide simply describes mathematical techniques for simulating subsurface air movement with ground-water modeling codes. As with any modeling study, the modeler must have a thorough understanding of site conditions with supporting data in order to properly apply the techniques presented in this guide.

6. Pressure-Squared Substitution Procedure

6.1 The pressure-squared substitution procedure is adapted from Baehr and Joss **(1)**. The technique allows simulation of the flow of gas (air in this case) through porous media using ground-water flow modeling codes. This is accomplished through substitution of air-phase parameters and variables into the ground-water flow equations. These substitutions are summarized as follows:

6.2 *Airflow Equation*—The following presentation outlines the essential assumptions of the airflow equation. A more detailed presentation providing justification of the various assumptions is provided by Baehr and Hult **(7)**.

6.2.1 The conservation of mass equation for airflow in an unsaturated porous medium is given by the following:

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla\cdot(\rho \sim q_s) = 0 \tag{1}$$

6.2.2 Darcy's Law for airflow is assumed as follows:

$$\sim q_s = -\frac{\rho g}{\mu} \approx k\,\nabla h \tag{2}$$

6.2.3 Hubbert (1940) defined the head for a compressible fluid as follows:

$$h = z + \frac{1}{g}\int_{P_0}^{P}\frac{1}{\rho}dP \tag{3}$$

6.2.4 The Ideal Gas Law is assumed to relate pressure and density and thus provides a model for air compressibility as follows:

$$\rho = \frac{\omega P}{RT} \tag{4}$$

6.2.5 Substituting Eq 4 into Eq 3, assuming ω and T are constant, neglecting the elevation component of head (that is small for air compared to the pressure component) and substituting into Eq 2 gives the following expression for Darcy's Law in terms of P:

$$\sim q_s = -\frac{1}{\mu} \approx k\,\nabla P \tag{5}$$

6.2.6 Substituting Eq 4 and Eq 5 into Eq 1, and then using the following linearizing change of variable suggested by Muskat and Botset **(8)** for airflow:

$$\phi = P^2 \tag{6}$$

yields the following three-dimensional airflow equation in Cartesian coordinates that is analogous in form to the ground-water flow equation solved by many ground-water flow models (MODFLOW **(9)**, for example):

$$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{yy}\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_{zz}\frac{\partial\phi}{\partial z}\right) = S_a\frac{\partial\phi}{\partial t} \tag{7}$$

where, x, y, and z are Cartesian coordinates aligned along the major axes of the permeability tensor with diagonal components k_{xx}, k_{yy}, and k_{zz}.

6.2.7 Air-phase permeability is assumed to be independent of P, therefore, the Klinkenberg slip effect **(10)** can only be modeled as constant with respect to P. The coefficient $S_a$is the pneumatic equivalent of specific storage and if air-filled porosity is constant with respect to time (that is, water movement is neglected) then:

$$S_a = \frac{\theta\mu}{\sqrt{\phi}} \tag{8}$$

6.2.8 The change of variable $\phi = P^2$ results in a linear equation for steady-state airflow. The transient equation is linearized by assuming $\phi^{1/2} = P_{atm}$ in the definition of S_a, where P_{atm} is the prevailing atmospheric pressure.

6.2.8.1 Massmann **(2)** describes the errors involved with the pressure-squared substitution described above, as well as simply substituting pressure for head. The error in the pressure-squared substitution is less than 1 % when the pressure difference between any two points in the flow field is less than 0.2 atmospheres (atm) and less than 5 % when the pressure difference is less than 0.8 atm. When substituting pressure (instead of pressure-squared) for head, the errors are similar for pressure differences less than 0.2 atm, but are quite large for pressure differences greater than 0.5 atm. In most cases, the pressure differences will be less than 0.2 atm; therefore, either substitution may be used in environmental modeling (see Section 7 for a description of the pressure substitution technique).

6.2.9 Eq 7 can be directly compared to the linear ground-water flow equation. The simplifying assumptions needed to arrive at this linear airflow equation are summarized as follows:

6.2.9.1 Darcy's law is valid for airflow;

6.2.9.2 The elevation component of pneumatic head is neglected;

6.2.9.3 Temperature effects are neglected;

6.2.9.4 The Ideal Gas law is a valid model for compressibility;

6.2.9.5 The Klinkenberg slip effect is neglected;

6.2.9.6 Water movement and consolidation are neglected, therefore porosity is constant with respect to time; and

6.2.9.7 $\phi^{1/2} = P_{atm}$ in definition of storage coefficient S_a.

6.2.10 Baehr and Hult **(7)** examined the consequences of the assumptions presented in 6.2.9. The authors found that the linear airflow model given by Eq 7 is a good working model for essentially all environmental applications.

6.3 *Ground-Water Flow Equation*—The following ground-water flow equation is solved by many ground-water flow models:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t} \tag{9}$$

where: x, y, and z are Cartesian coordinates aligned along the major axes of the hydraulic conductivity tensor with diagonal components K_{xx}, K_{yy}, K_{zz}.

6.3.1 The purpose of the procedure presented in this guide is to facilitate airflow simulations by matching Eq 7 and Eq 9 so that the numerical solution coded in ground-water flow models can be used to solve the airflow equation. This is accomplished with the following parameter matches:

$$h \Rightarrow \phi \tag{10}$$

$$K \Rightarrow k \tag{11}$$

$$S_s \Rightarrow S_a \tag{12}$$

6.3.2 The parameter matching allows the hydraulic head and flow output from the ground-water model to be interpreted for the airflow model in accordance with 6.3.

6.4 *Boundary Conditions*—There are only two permissible types of boundary conditions when using the pressure-squared substitution described above. These include constant pressure and no-flow boundaries.

6.4.1 Constant pressure cells are actually constant pressure-squared cells. Constant pressure cells are used in two ways:

6.4.1.1 Constant pressure cells are set around the perimeter of the model to allow air to flow into the model horizontally, and

6.4.1.2 Venting wells and trenches are defined as constant pressure cells where the pressure is the absolute pressure (squared) maintained in the venting well.

6.4.2 An extra layer of constant pressure cells should be added at the top of the model domain to simulate the connection between the vadose zone and the atmosphere. The cells in this top layer and the constant pressure cells around the outside of the model are maintained at the prevailing atmospheric pressure (squared). To make sure that the model covers a sufficiently large area around the venting system, at least 90 % of the air inflow to the model should come from the top atmospheric layer (as opposed to the lateral edges of the model) **(1)**.

6.4.3 Wells and trenches should be maintained at a constant value of ϕ. The ground-water flow model will then compute a flow rate (q^*) that must be transformed to a volumetric airflow rate (q_v) or mass flow rate (q_m) in accordance with Eq 18 and Eq 21, respectively.

6.4.4 No-flow boundaries are normally prescribed along the base of the model representing the water table or boundary with the saturated aquifer system. No-flow cells may also be used to represent foundations, paved areas, or other subsurface material impermeable to air.

6.5 *Interpretation of Model Head Output*—As a result of the parameter matches discussed in 6.2, cell values of $\phi = P^2$ will be computed by the ground-water flow model. Taking the square root of the head output values gives the pressure distribution for the airflow simulation.

6.6 *Interpretation of Model Flow Output*—Ground-water flow models compute cell by cell components of flow vectors that need to be interpreted to obtain airflow rates. Most ground-water flow modeling codes (MODFLOW **(9)**, for example) calculate components of airflow rates as follows:

$$q = -KA\frac{\partial h}{\partial l} \tag{13}$$

6.6.1 Based on the transformations given by Eq 10 and Eq 11, flow output corresponds to the following terms for an airflow simulation:

$$q^* = -kA\frac{\partial \phi}{\partial l} \tag{14}$$

where: q^* is the flow term computed by the model and related to airflow in units g^2-cm/s^4.

6.6.2 To relate q^* to air flow, recognize that:

$$\frac{\partial \phi}{\partial l} = \frac{\partial (P^2)}{\partial l} = 2P\frac{\partial P}{\partial l} \tag{15}$$

6.6.3 Substituting Eq 15 into 14 gives:

$$q^* = 2kAP\frac{\partial P}{\partial l} \tag{16}$$

6.6.4 From Eq 5, Darcy's Law for volumetric airflow is as follows:

$$q_v = \frac{kA\partial P}{\mu\ \partial l} \tag{17}$$

6.6.5 Therefore, the ground-water model flow output q^* is converted as follows:

$$q_v = q^*\left(\frac{1}{2\mu\sqrt{\phi}}\right) \tag{18}$$

6.6.6 Therefore to obtain components of volumetric airflow, the head output file must be combined with the flow output as indicated by Eq 16 Eq 17 Eq 18.

6.6.7 Mass air flow rate is given by:

$$q_m = \rho q_v \tag{19}$$

6.6.8 Substituting the ideal gas law, Eq 4 into Eq 19 and then substituting into Eq 17, yields the following

$$q_m = -kAP\frac{\omega\ \partial P}{\mu RT\partial l} \tag{20}$$

6.6.9 Therefore, q_m is given as follows:

$$q_m = q^*\left(\frac{\omega}{2\mu RT}\right) \tag{21}$$

6.6.10 Therefore to obtain components of mass airflow, the ground-water flow output values for q^* is multiplied by the term appearing in Eq 21.

7. Pressure Substitution Procedure

7.1 The pressure substitution technique is adapted from Massmann **(2)** and is simpler to apply than the pressure-squared substitution technique. As stated in 6.8.2.1 , however, the pressure substitution technique is only valid when the pressure difference between any two points in the system is less than about 0.2 atm.

7.2 The pressure substitution technique makes the following substitutions into Eq 9 (the ground-water flow equation):

$$K = \frac{\rho g k}{\mu} \tag{22}$$

$$S_s = \frac{g\omega\theta}{RT}$$

$$h = \frac{P}{\rho g}$$

7.3 These substitutions are straightforward; however, gas composition is often unknown. In that case, the density (ρ), viscosity (μ), and molecular weight (ω) of air may be assumed as follows:

7.3.1 ρ (air) = 1.3×10^{-3} g/cm^3.

7.3.2 μ (air) = 1.8×10^{-4} g/cm/s (0.018 cP).

7.3.3 ω (air) = 28 g/mol.

7.3.4 Also note that g = 980 cm/s^2 and k may be obtained from estimates of saturated hydraulic conductivity as $k = 1.02 \times 10^{-5}K$.

8. Keywords

8.1 airflow; computer model; ground water; simulation; soil venting

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