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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.

[1] This guide is under the jurisdiction of ASTM Committee D18 on Soil and Rock and is the direct responsibility of Subcommittee D18.21 on Ground Water and Vadose Investigations.

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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.

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

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)**.