DOCUMENTATION OF AIR2D, A COMPUTER PROGRAM TO SIMULATE TWO-DIMENSIONAL AXISYMMETRIC AIR FLOW IN THE UNSATURATED ZONE

By Craig J. Joss and Arthur L. Baehr

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COMPUTER CODE AVAILABILITY

The computer program for AIR2D and example data sets are contained on the diskette provided with this report. The computer program and example data sets are also available through the World-Wide Web at the following address:

http://wwwnj.er.usgs.gov .

CONTENTS

CONTENTS--Continued

REFERENCES

ATTACHMENTS

In pocket--Diskette containing the following:
An instructional narrative file
Fortran source file for program AIR2D.FOR
Executable versions of above codes using a Microsoft[1] Fortran compiler
and IBM-compatible computer

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[1] Use of trade names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

ILLUSTRATIONS

ILLUSTRATIONS--Continued

CONVERSION FACTORS

MULTIPLY	BY	TO OBTAIN
	Length	
inch (in)	2.54	centimeter (cm)
	Mass	
pound (lb)	2204.6	gram (g)
	Time	
second (s)	1.1574×10^{-5}	day (d)
	Air-Phase Permeability	
darcy (drcy)	1.0×10^{-8}	square centimeter (cm^2)
	Pressure	
atmosphere (atm)	760.0	millimeters of mercury (mm-Hg)
atmosphere (atm)	406.794	inches of water (in-H_2O)
atmosphere (atm)	101.325	kilo-Pascal (k-Pa)
atmosphere (atm)	14.696	pounds per square inch (lb/in^2)
	Temperature	
degree Celsius = C	degree Kelvin = K	degree Fahrenheit = F

$C=K-273.15$

$F=1.8C + 32$

$C=(F-32)/1.8$

DOCUMENTATION OF AIR2D, A COMPUTER PROGRAM TO SIMULATE TWO-DIMENSIONAL AXISYMMETRIC AIR FLOW IN THE UNSATURATED ZONE

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ABSTRACT

This report presents a flow model that simulates the movement of air to or from a single borehole screened in the unsaturated zone. The model can be applied to predict the flow field associated with vapor extraction, a popular method for removing volatile organic compounds spilled in the subsurface. An axisymmetric unsaturated domain and steady-state conditions are assumed. The model has two analytical solution options--one for a domain connected directly to the atmosphere and one for a domain separated from the atmosphere. The air-flow models have been incorporated into a computer program called AIR2D. AIR2D can be used in a calibration mode to obtain estimates of unsaturated zone air-phase permeability from pneumatic pump test data. Alternatively, AIR2D can be used in a prediction mode to simulate the performance of a single venting well by generating pressure and flow values for a specified geologic setting, air permeability distribution, and well discharge or injection rate.

Two field procedures are presented for performing pneumatic pump tests, a full-scale permeability test and a small-scale permeability test. In the full-scale test, pressure measurements are taken at multiple locations in the unsaturated zone. The data set then can be used to generate horizontal and vertical air permeability estimates for the model domain, and if applicable, the air permeability of an overlying lithologic unit of lower air permeability, which acts as a confining unit. In the small-scale permeability test, a single pressure value at the well screen is determined by measuring the system pressure at the surface and correcting the measured value for pressure losses due to friction in the pipe. These data can be used to generate a composite air-permeability estimate under the assumption of domain isotropy. AIR2D has the capability of analyzing data sets from both types of pneumatic pump test.

AIR2D is written in Fortran '77 and, with minor modifications, will run on both personal and mainframe computers. The computer program for AIR2D and example data sets are contained on the diskette provided with this report. The computer program is also available through the World-Wide Web at the following address: http://wwwnj.er.usgs.gov .
The program is menu driven and runs from data files created or modified by using the editing options in AIR2D.

SECTION 1.0--INTRODUCTION AND USER'S GUIDE

Government regulators and the public have become increasingly aware of the contamination of soil and ground water by volatile organic compounds. This increased awareness has led to the development of methods that improve the performance of remediation systems. A technology known as vapor extraction or soil venting has emerged as an effective technique for the remediation of soils contaminated with volatile organic compounds. Although vapor extraction is relatively simple in concept, the air-flow pattern induced by venting can be complex. The efficiency of the remediation system depends directly on the amount of air flow that intersects the contaminant plume; therefore, some means of quantifying air flow is needed. Baehr and Hult (1991) developed an analytical solution to the air-flow equation that describes the steady-state movement of air to or from a well that partially penetrates the unsaturated zone of the domain open to the atmosphere. This solution is implemented by AIR2D.

Baehr and Hult (1991) developed another analytical solution for situations where the domain is separated from the atmosphere by a confining unit. A modified solution based on the well hydraulics solution presented by Hantush (1967) has been developed by Baehr and Joss (1995) and also is implemented by AIR2D. AIR2D is a tool that can be used to apply basic scientific principles to the design vapor extraction systems.

This report documents the software package called AIR2D, which computes pressure and flow in an axisymmetric domain under steady-state conditions for either geologic condition, domain open to the atmosphere or domain separated from the atmosphere. Examples of data input and output for each program application are presented. Detailed descriptions of the file layouts and contents of each program application also are presented. The computer program for AIR2D and example data sets are contained on the diskette provided with this report. The computer program is also available through the World-Wide Web at the following address: http://wwwnj.er.usgs.gov .

Section 2 presents a theoretical overview of the two air-flow modeling options. The first option, Open, applies to a domain connected directly to the atmosphere and assumes that a water table or impermeable unit forms the lower (no flow) boundary. The second option, Hantush, applies to a domain separated from the atmosphere by a confining unit and simulates air movement through the confining unit from the upper boundary. For the second solution, a water table or impermeable unit forms the lower (no flow) boundary.

The air-flow model can be implemented in either a calibration or a prediction mode. In the calibration mode, the model is used to estimate the air-phase permeability of the unsaturated zone from data collected during a pneumatic pump test. Two field procedures--a full-scale pneumatic pump test and a small-scale pneumatic pump test--are discussed in Section 3. The full-scale permeability analysis involves injecting or withdrawing air through a well screened in the unsaturated zone. The resulting pressure distribution, at steady state, can be measured by using a network of probes surrounding the well. When the pressure at specific points in the domain and the mass flow rate at the well are known, the horizontal (k_r) and vertical (k_z) components of air-phase permeability can be estimated by calibrating the governing model with AIR2D. If applicable, the air permeability of the upper unit (k') can be estimated. Alternatively, the small-scale permeability analysis involves injecting or withdrawing air through a vapor probe located in the unsaturated zone. The well-head pressure measurement then is used to determine the pressure at the probe screen by correcting for friction losses in the system. When the pressure at the probe and the air-flow rate at the well are known, the composite permeability can be estimated by calibrating the air-flow model with AIR2D. The small-scale permeability technique is equivalent conceptually to performing a full-scale permeability test with a single pressure measurement in the domain. The small-scale permeability technique was developed to take advantage of site instrumentation, that was installed to conduct soil-gas surveys and that typically consists of narrow tubing.

AIR2D also contains an option to estimate the friction factor that correspond to air flow in a pipe. This is a required input value in the small-scale permeability analysis. The friction factor can be obtained from either experimental results or theoretical considerations. A brief overview of both approaches is presented and experimental and theoretical friction factors are compared in Section 3.

In the prediction mode, the models can be used to estimate pressure distribution values in the domain, air-flow paths and air-flow rates for a given geologic setting, and well discharge or injection rates. Because contaminant removal is proportional to air-flow rates, the models can be used to design venting systems. In addition, the effects of low-permeability caps and different screen intervals can be investigated with AIR2D.

For applications requiring a full three-dimensional analysis, the user is referred to the companion model AIR3D (Joss and Baehr, 1995). Use of the total software package, AIR2D and AIR3D, involves multiple applications of AIR2D to determine air-permeability distribution. The permeability-distribution value is then used in AIR3D for a rigorous simulation of air flow through multiple wells or trenches at a heterogeneous site.

An overview of the program AIR2D is presented in Section 4. With minor modifications, the program can be run on a variety of computer systems, including personal and mainframe computers. The program is menu-driven and provides options for either calibration or prediction applications. In order to implement the program, input must be provided in data files. AIR2D provides an editing option for creating and modifying the required input files. Alternatively, a text editor can be used to create the necessary input files or modify existing files. Detailed descriptions of the file layouts and contents for each program application are presented. Output from AIR2D calibration runs is displayed on the computer screen, and, if specified by the user, will be written to output files. Output from AIR2D prediction runs are written to separate pressure, volumetric flow, mass flow, and well output files. The components and flow of information in AIR2D are shown in figure 1. The TESTxx data file will vary according to model applications. The CALIB data file is required only when flow measurements are entered into AIR2D in terms of flowmeter scale readings. The FRIC data file is required only for small-scale permeability analyses. Descriptions of the data files can be found in Section 4.

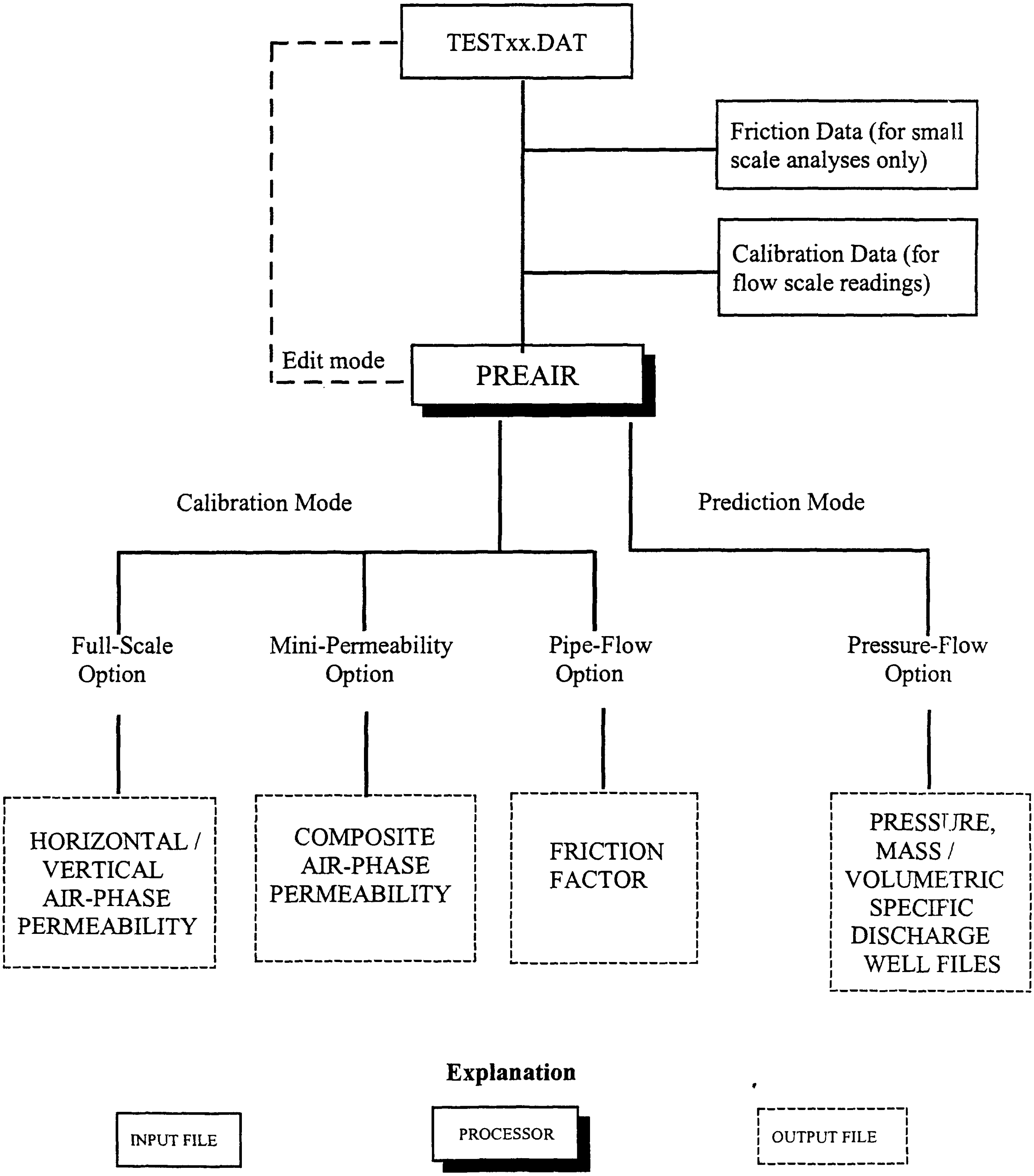

Figure 1. Components and flow of information in the AIR2D software package.

The diskette provided with this document contains the following files:

README - an instructional narrative (ASCII text file),
AIR2D.FOR - Fortran source code for air-flow model,
AIR2D.EXE - AIR2D executable file,
DATA FILES - examples of AIR2D applications illustrated in Sections 4.2, 4.3, 4.4, and 4.5.

Note that the executable files were created by compiling the corresponding Fortran codes on an IBM-compatible personal computer with a Microsoft[1] Fortran compiler.

Users with access to Fortran compilers are encouraged to compile the source code. The executable version of the code provided on the diskette (AIR2D.EXE) is intended only for users who do not have access to a Fortran compiler. To install AIR2D on a computer with a Fortran compiler, the installation and execution procedure is as follows:

1. Copy files from diskette to the computer.

2. Rename the source-code file so that it has the extension required by the Fortran compiler, for example, for a mainframe, AIR2D.F77, for a personal computer, AIR2D.FOR.

3. Check input and output unit-number settings in AIR2D for compatibility with either mainframe or personal computer. The sections of code that define these units are clearly identified in the source codes and are defined in the reference manual. (See Section 4.1.4 for instructions.)

4. Compile the source code. For example, the command for the Microsoft Fortran compiler is FL AIR2D.FOR.

5. Run an AIR2D simulation by first creating the data-input file required to define the simulation:

   TEST1x - full-scale permeability data file (see Section 4.2.1),
   TEST2x - small-scale permeability data file (see Section 4.3.1),
   TEST3a - experimental friction factor data file (see Section 4.4.1),
   TEST3b - theoretical friction factor data file (see Section 4.4.2),
   TEST4x - pressure / flow prediction data file (see Section 4.5.1).

   Then, execute the program AIR2D. For example, the command to run AIR2D on a personal computer is AIR2D.

Users are encouraged to test their understanding of the AIR2D software package by performing test simulations with the data files provided.

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SECTION 2.0--AIR-FLOW MODELING

2.1 Overview of Air-flow Modeling

Simulating air movement in porous media historically has been an important area of research in the petroleum industry. Pioneering work in this area was performed by Muskat and Botset (1931), who developed a one-dimensional (radial) air-flow model to evaluate the horizontal permeability of gas reservoirs. Air-flow models also have been used to evaluate the permeability of other formations. Boardman and Skrove (1966) injected air into isolated sections of test holes and measured pressure distributions at radial distances to obtain the value of horizontal permeability of fractured granitic rock. Weeks (1977) describes the use of atmospheric variations in air pressure to calculate the distribution of vertical air permeability of the unsaturated zone. Massman (1989) adapted the Theis solution for one-dimensional radial ground-water flow to a well to predict pressure drawdown with a vapor extraction well. However, a one-dimensional model poses serious limitations in evaluating air-permeability distribution. Baehr and Hult (1988) presented two-dimensional analytical solutions for transient air flow to a well. However, their derivation required that the well be modeled as an infinitesimal line source. The steady-state solutions presented here allow for a well of finite radius, which can be an important modeling capability for the simulation of a small-scale permeability pneumatic test.

Numerical models for simulating gas flow in the unsaturated zone have been developed recently by Wilson and others (1987), Metcalf and Farquhar (1987), Pruess (1987), Wilson and others (1988), Baehr and Hult (1988), Sleep and Sykes, (1989), Falta and others (1989), Thorstenson and Pollack (1989), Mendoza and Frind (1990), and Baehr and Bruell (1990). Despite these developments, further refinements to the models are needed to facilitate the design vapor extraction systems.

2.2 Air-Flow Equation

The theory of compressible fluid flow in unsaturated porous media, as presented by Baehr and Hult (1991), is outlined in this section to provide the user with an understanding of the model assumptions leading to the basic air-flow equation.

The air-flow equation for an unsaturated porous medium is derived by applying several basic equations. The derivation starts with the conservation of mass equation for air flow in an unsaturated porous medium which is given by:

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla\cdot(\rho \underset{\sim}{q}) = 0 \qquad (1)$$

where

ρ = density of the air [g/cm^3]
θ = air-filled porosity [-]
t = time [s]
$\underset{\sim}{q}$ = specific-discharge vector for air [cm/s]

Darcy's Law for air flow is assumed and is written as follows:

$$\underset{\sim}{q} = -\frac{\rho g}{\mu} \underset{\approx}{k} \nabla h \qquad (2)$$

where

μ =	dynamic viscosity of air	[g/cm-s]
g =	acceleration due to gravity	[cm/s^2]
h =	air-phase potential head	[cm]
$\underset{\approx}{k}$ =	air-phase permeability tensor	[cm^2]

In the most general case, $\underset{\approx}{k}$ should be regarded as a tensor; however, here it is assumed that the coordinate system is aligned with the principal axes with respect to air-phase permeability.

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

$$h = z + \frac{1}{g} \int_{Po}^{P} \frac{1}{\rho} dP \qquad (3)$$

where, for the air phase in the unsaturated zone,

z =	elevation head	[cm]
P =	air-phase pressure	[$g/cm\text{-}s^2$]
P_0 =	reference air-phase pressure	[$g/cm\text{-}s^2$]

The ideal gas law is assumed to relate pressure and density and thus provides a model for air compressibility as follows:

$$\rho = \frac{\omega P}{RT} \qquad (4)$$

where

ω =	average molecular weight of air phase (that is 28.8)	[g/mol]
R =	universal gas constant = 8.314×10^7	[$g\text{-}cm^2/s^2\text{-}mol\text{-}K$]
T =	temperature	[K]

By substituting equation (4) into equation (3), assuming ω and T are constant, neglecting the elevation component of head, and substituting the result into equation (2), the following expression for Darcy's Law in terms of P is obtained.

$$\underset{\sim}{q} = -\frac{1}{\mu} \underset{\approx}{k} \nabla P \qquad (5)$$

Substituting equations (4) and (5) into equation (1), using the following linearizing change of variable suggested by Muskat and Botset (1931) for air flow:

$$\phi = P^2 \qquad (6)$$

and making the additional assumptions discussed below, the following transient air-flow equation for axisymmetric flow is obtained.

$$\mu\theta \frac{1}{\sqrt{\phi}} \frac{\partial\phi}{\partial t} = k_r \frac{\partial^2\phi}{\partial r^2} + k_r \frac{1}{r} \frac{\partial\phi}{\partial r} + k_z \frac{\partial^2\phi}{\partial z^2} \qquad (7)$$

where

r and z are polar coordinates aligned along the major axes of the air permeability k_r and k_z

ϕ = pneumatic pressure squared term [$(g/cm\text{-}s^2)^2$]

t = time [s]

The right-hand side of equation (7) is linear in ϕ and, therefore, amenable to analytical solution. In obtaining equation (7), the following additional assumptions were made (refer to Baehr and Hult, 1991):

- the elevation component of head is neglected;
- air-filled porosity, temperature, and average molecular weight for air are assumed to be constant;
- domain is assumed to be homogeneous with respect to k_r and k_z;
- the Klinkenberg Slip Effect is modeled as an averaged effect and does not depend on the air-pressure gradient.

Under these assumptions and assuming that a well has an infinitesimal diameter, Baehr and Hult (1988) developed an analytical solution to equation (7) for both transient and steady-state cases. The assumption that a well has an infinitesimal diameter is necessary to obtain a transient solution. If only the steady-state air-flow equation

$$k_r \frac{\partial^2\phi}{\partial r^2} + k_r \frac{1}{r} \frac{\partial\phi}{\partial r} + k_z \frac{\partial^2\phi}{\partial z^2} = 0 \qquad (8)$$

is considered, analytical solutions exist for the case of a well with finite diameter (see Baehr and Hult,1991).

Only steady-state analysis is required to determine air permeability. The finite diameter well modeling capability is important for small-scale field tests and for simulating the effects of high permeability gravel packs.

2.3 Analytical Solutions Programmed in AIR2D

AIR2D implements two analytical solutions to the steady-state air-flow equation (8). Each corresponds to the characteristic of the top horizontal boundary condition. The two alternatives are

(1) the top of the domain is in direct contact with the atmosphere, and pressure is set at atmospheric pressure, which represents a first kind boundary condition, and

(2) the domain is separated from the atmosphere by a confining unit which is modeled by using a third-kind boundary condition.

The derivation of solution 1 is presented by Baehr and Hult (1991). The derivation of solution 2 is presented by Baehr and Joss (1995) and emulates the well-hydraulics solution of Hantush (1967).

2.3.1 Solution for a Domain Connected Directly to the Atmosphere

A schematic of the model domain is shown in figure 2. The top of the unsaturated zone is assumed to be in direct connection with the atmosphere. The bottom boundary is formed by the water table or an impervious unit. The analytical solution to equation (8) from Baehr and Hult (1991) is as follows:

$$\phi = P^2_{atm} + \frac{2aQ^*}{\pi^2 k_r (l-d) r_w} \tag{9}$$

$$\left\{ \sum_{n=1}^{\infty} \frac{1}{m} \left[\frac{\cos\left(\frac{m\pi d}{b}\right) - \cos\left(\frac{m\pi l}{b}\right)}{M_m K_1 \left(M_m \frac{r_w}{a}\right)} \right] K_0 \left(M_m \frac{r}{a}\right) \sin\left(M_m z\right) \right\}$$

where

ϕ = air pressure squared [$(g/cm\text{-}s^2)^2$]
P_{atm} = atmospheric pressure [$g/cm\text{-}s^2$]
Q = constant mass flow rate [g/sec]
$Q^* = \frac{Q\mu RT}{\omega}$
μ = dynamic viscosity of air [g/cm-sec]
R = universal gas constant = 8.3143×10^7 [$g\text{-}cm^2/s^2\text{-}mol\text{-}K$]
T = absolute temperature [K]
ω = average molecular weight of air phase [g/mol]
k_r = horizontal air permeability [cm^2]
k_z = vertical air permeability [cm^2]
a = square root of anisotropy ratio $(k_r/k_z)^{1/2}$ [-]
r_w = radius of the well (to filter/soil interface) [cm]
r = radial distance from well center line [cm]

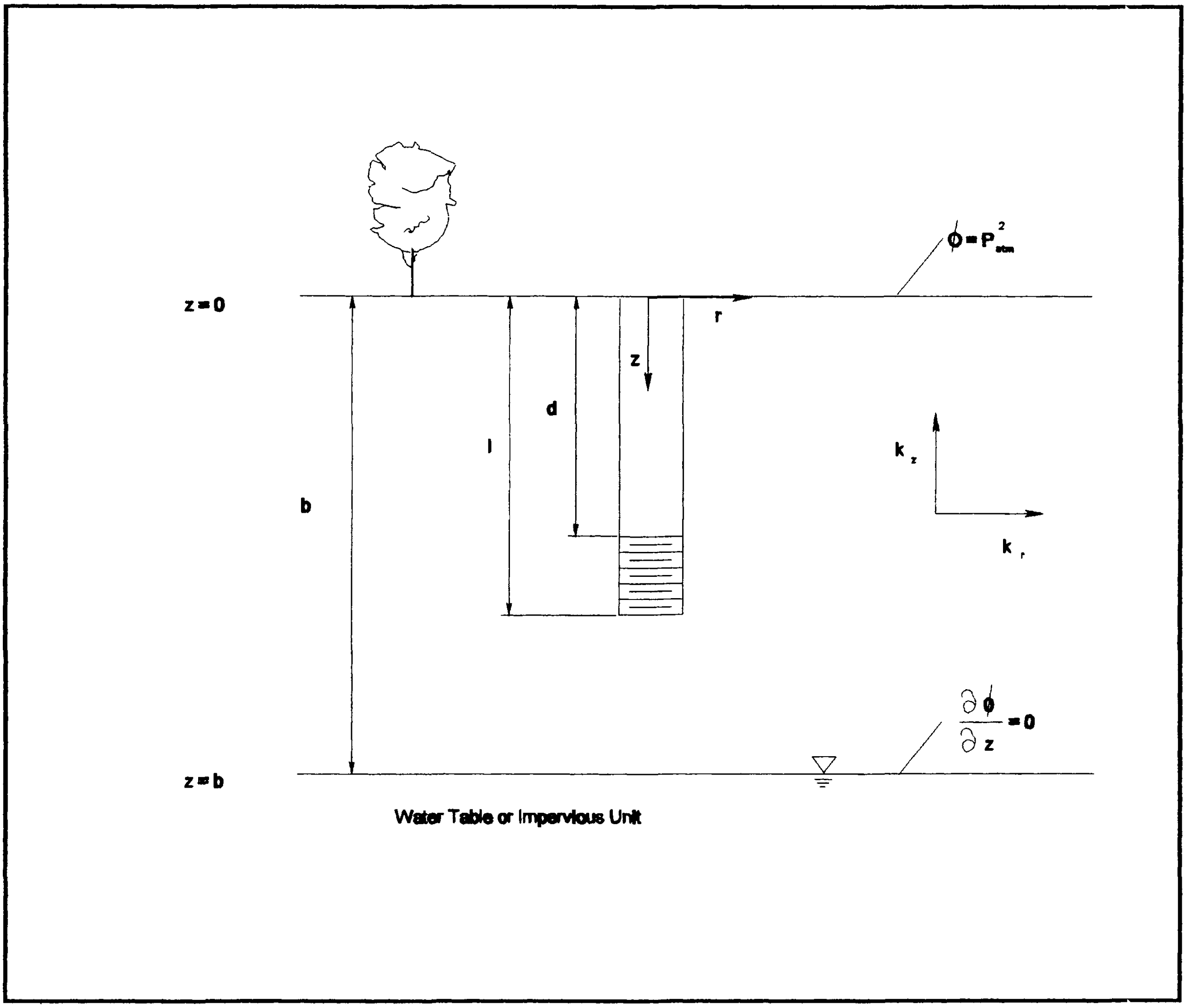

Figure 2. Domain connected directly to the atmosphere.

z = vertical distance from land surface [cm]
b = vertical thickness of domain (see figure 2) [cm]
d = distance from land surface to top of the well screen (see figure 2) [cm]
l = distance from land surface to bottom of the well screen (see figure 2) [cm]

and

$m = n - \frac{1}{2}$
K_0 = zero order modified Bessel function of the second kind
K_1 = first order modified Bessel function of the second kind
$M_m = \left(\frac{m\pi}{b}\right)$

Equation (9) gives pressure at any point (r,z) in the model domain. Equation (9) is differentiated as shown below to obtain analytical expressions for the pressure gradient used to define specific discharge.

$$\frac{\partial\phi}{\partial r} = \frac{-K}{a}\left\{\sum_{n=1}^{\infty} M_m\, \alpha_m \sin(M_m z)\, K_1\!\left(M_m \frac{r}{a}\right)\right\} \tag{10}$$

$$\frac{\partial\phi}{\partial z} = \frac{\pi K}{b}\left\{\sum_{n=1}^{\infty} m\, \alpha_m \cos(M_m z)\, K_0\!\left(M_m \frac{r}{a}\right)\right\} \tag{11}$$

where

$$K = \frac{2aQ^*}{\pi^2 k_r (l-d) r_w}$$

$$\alpha_m = \frac{1}{m}\left[\frac{\cos(M_m d) - \cos(M_m l)}{M_m K_1\left(M_m \frac{r_w}{a}\right)}\right]$$

Volumetric specific discharge in the horizontal (r) and vertical (z) directions are obtained by combining equations (10) and (11) with Darcy's Law, equation (5), and are given as follows:

$$q_{rv} = -\frac{k_r}{2\,\mu\,\sqrt{\phi}}\;\frac{\partial\phi}{\partial r} \tag{12}$$

$$q_{zv} = -\frac{k_z}{2\,\mu\,\sqrt{\phi}}\;\frac{\partial\phi}{\partial z} \tag{13}$$

where

q_{rv} = volumetric specific discharge in horizontal direction [cm/s]
q_{zv} = volumetric specific discharge in vertical direction [cm/s]

The factor $2\sqrt{\phi}$ that appears in equations (12) and (13) results from the substitution of $\phi=P^2$ into

Darcy's Law, equation (5).

Mass specific discharge in the horizontal and vertical directions is obtained by multiplying volumetric specific discharge by density, given by equation (4), as follows:

$$q_{rm} = - \frac{\omega\, k_r}{2\, \mu\, R\, T} \frac{\partial \phi}{\partial r} \qquad (14)$$

$$q_{zm} = - \frac{\omega\, k_z}{2\, \mu\, R\, T} \frac{\partial \phi}{\partial z} \qquad (15)$$

where

q_{rm} = mass specific discharge in horizontal direction [g/cm^2-s]

q_{zm} = mass specific discharge in vertical direction [g/cm^2-s]

In the above equations, $(\partial\phi/\partial r)$ is given by equation (10) and $(\partial\phi/\partial z)$ is given by equation (11). The flow rates also can be integrated over horizontal and vertical surfaces in the domain to obtain net flow through two-dimensional sections in the model.

The mass flow rate in the horizontal direction, through a vertical two-dimensional surface (that is a cylindrical face) at radius r_c, is obtained by integrating over two pi radians between a lower (z_1) and upper (z_2) depth, as follows:

$$Q_{rm} = 2\, \pi\, r_c \int_{z_1}^{z_2} q_{rm}\; dz \qquad (16)$$

where

Q_{rm} = mass flux in r-direction across vertical control face [g/s]

The mass flow rate in the vertical direction, through a horizontal two-dimensional surface (that is, a disk) at depth z_c, is obtained by integrating over two pi radians between an inner (r_1) radius and outer (r_2) radius, as follows:

$$Q_{zm} = 2\, \pi \int_{r_1}^{r_2} q_{zm}\; r\; dr \qquad (17)$$

where

Q_{zm} = mass flux in z-direction across horizontal control face [g/s]

The quantities defined by equations (16) and (17) are interpreted in normalized terms by dividing mass flow rate by the total mass flow through the well, as follows:

$$F_{tot} = \frac{Q_m}{Q_{well}} \times 100 \qquad (18)$$

where

F_{tot}	= percent of total mass passing through a two-dimensional section	[%]
Q_m	= mass flow rate passing through a two-dimensional section (Q_{rm} or Q_{zm})	[g/s]
Q_{well}	= total mass flow rate through a well	[g/s]

By substituting equations (10) and (14) into equation (16) and integrating between the limits z_1 and z_2 at radius r_c over two pi radians, the following solution to horizontal mass flow through a vertical two-dimensional surface is obtained.

$$Q_{rm}(r_c,z_1,z_2) = \frac{r_c\ \omega\ k_r\ K\ b}{\mu\ R\ T\ a} \left\{ \sum_{n=1}^{\infty} \frac{M_m\ \alpha_m}{m} K_1\left(M_m \frac{r_c}{a}\right) \left[\cos\left(M_m z_1\right) - \cos\left(M_m z_2\right) \right] \right\} \qquad (19)$$

By substituting equations (11) and (15) into equation (17) and integrating between the limits r_1 and r_2 at depth z_c over two pi radians, the following solution to vertical mass flow through a horizontal two-dimensional surface is obtained.

$$Q_{zm}(z_c,r_1,r_2) = \frac{-\pi^2\ \omega\ k_z\ K\ a}{\mu\ R\ T\ b} \left\{ \sum_{n=1}^{\infty} \frac{m\ \alpha_m}{M_m} \cos\left(M_m z_c\right) \left[r_2\ K_1\left(M_m \frac{r_2}{a}\right) - r_1\ K_1\left(M_m \frac{r_1}{a}\right) \right] \right\} \qquad (20)$$

Equations (19) and (20) provide estimates of the mass flow rate through vertical and horizontal two-dimensional sections in the model domain. By incorporating the above results into equation (18), flow through the surfaces can be represented as a percentage of the total flow out of the well.

2.3.2 Solution for a Domain Separated From the Atmosphere by A Confining Unit

A schematic of the model domain is shown in figure 3. The upper, leaky confining unit consists of a strata less permeable to air than the domain. The bottom boundary is formed by the water table or an impervious unit. This solution simulates flow through the unit by using a third-kind boundary condition, as suggested by Hantush (1967). Baehr and Joss (1995) present the derivation of the solution for air flow, which is obtained by using a generalized cosine transformation. The solution is as follows:

$$\phi = P_{atm}^2 + \frac{2\,h\,Q^*\,a\,b}{\pi\,k_r(l-d)r_w} \tag{21}$$

$$\left\{ \sum_{n=1}^{\infty} \left[\frac{\sin\left(q_n \frac{b-d}{b}\right) - \sin\left(q_n \frac{b-l}{b}\right)}{q_n^2\;K_1\left(\frac{q_n r_w}{b\,a}\right)} \right] \left[\frac{\cos\left(q_n \frac{b-z}{b}\right)}{h + \sin^2 q_n} \right] K_0\left(\frac{q_n r}{a\,b}\right) \right\}$$

where

q_n, n=1,2,3,... are the positive solutions to $\tan(q_n) = h/q_n$

and

h	$= (k'b/k_z b')$	[-]
k_r	= horizontal permeability of the air phase	[cm^2]
k_z	= vertical permeability of the air phase	[cm^2]
k'	= permeability of upper unit	[cm^2]
b'	= thickness of upper unit	[cm]

In AIR2D the solutions q_n are obtained numerically by using the Newton-Raphson iteration.

Pressure gradients are given by:

$$\frac{\partial\phi}{\partial r} = \frac{-K}{ab}\left\{ \sum_{n=1}^{\infty} q_n\,\alpha_n \cos\left(q_n\left(\frac{b-z}{b}\right)\right) K_1\left(\frac{q_n r}{a\,b}\right) \right\} \tag{22}$$

and

$$\frac{\partial\phi}{\partial z} = \frac{K}{b}\left\{ \sum_{n=1}^{\infty} q_n\,\alpha_n \sin\left(q_n\left(\frac{b-z}{b}\right)\right) K_0\left(\frac{q_n r}{a\,b}\right) \right\} \tag{23}$$

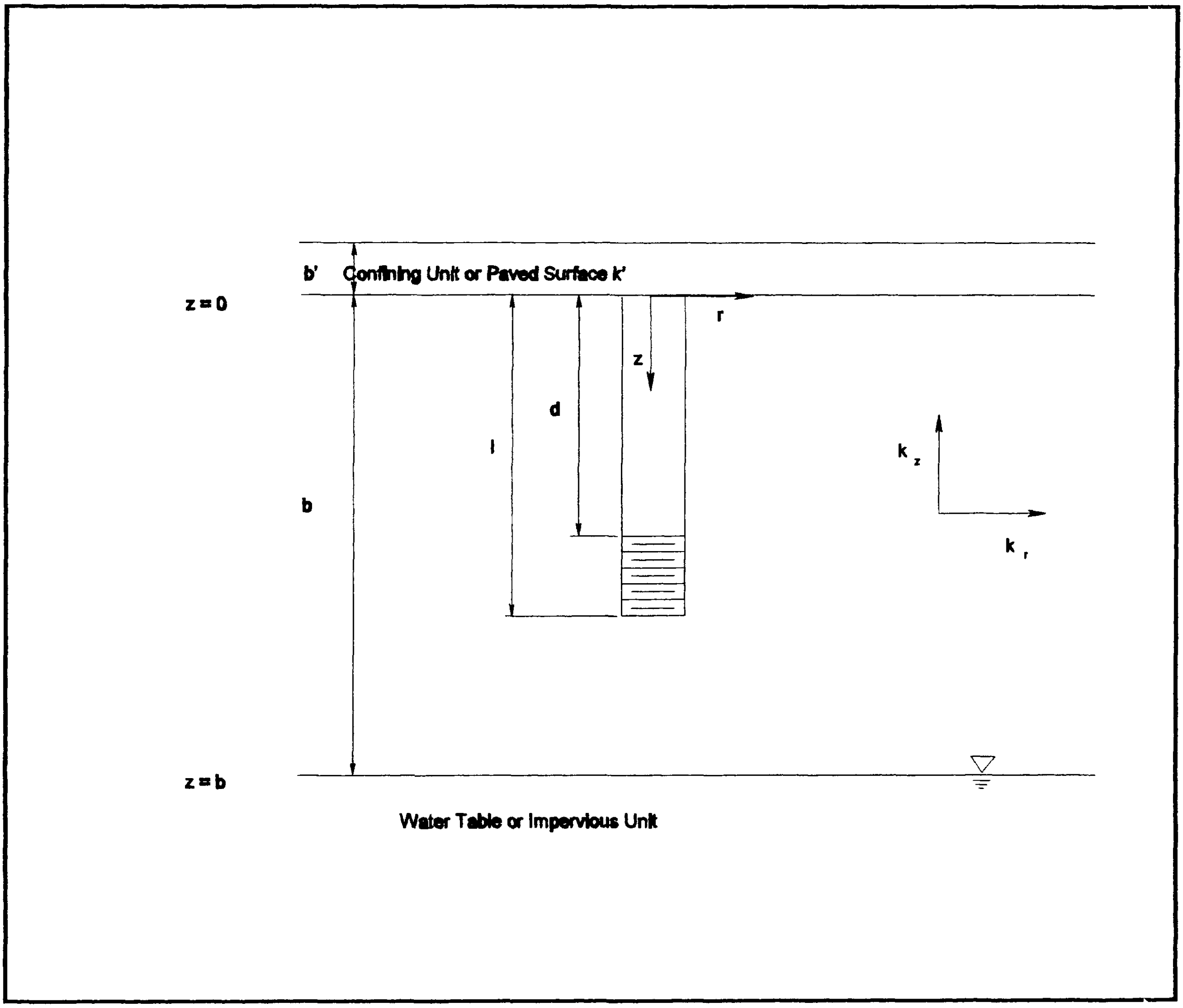

Figure 3. Domain separated from the atmosphere by a confining unit.

where

$$K = \frac{2 h Q^* a b}{\pi k_r (l-d) r_w}$$

$$\alpha_n = \left[\frac{\sin\left(q_n \frac{b-d}{b}\right) - \sin\left(q_n \frac{b-l}{b}\right)}{q_n^2 K_1\left(\frac{q_n r_w}{a b}\right)\left(h + \sin^2 q_n\right)} \right]$$

Specific discharge components are obtained by substituting equations (22) and (23) into equations (12) through (15). By substituting equations (22) and (14) into equation (16) and integrating between the limits z_1 and z_2 at radius r_c over two pi radians, the solution to horizontal mass flow through a vertical two-dimensional surface is obtained.

The horizontal mass flow solution is as follows:

$$Q_{rm}(r_c, z_1, z_2) = \frac{\pi r_c \omega k_r K}{\mu R T a} \left\{ \sum_{n=1}^{\infty} \alpha_n K_1\left(\frac{q_n r_c}{a b}\right) \left[\sin\left(q_n \frac{b-z_1}{b}\right) - \sin\left(q_n \frac{b-z_2}{b}\right) \right] \right\} \qquad (24)$$

By substituting equations (23) and (15) into equation (17) and integrating between the limits r_1 and r_2 at depth z_c over two pi radians, the following solution to vertical mass flow through a horizontal two-dimensional surface is obtained.

$$Q_{zm}(z_c, r_1, r_2) = \frac{-\pi \omega k_z K a}{\mu R T} \left\{ \sum_{n=1}^{\infty} \alpha_n \sin\left(q_n \frac{b-z_c}{b}\right) \left[r_2 K_1\left(\frac{q_n r_2}{a b}\right) - r_1 K_1\left(\frac{q_n r_1}{a b}\right) \right] \right\} \qquad (25)$$

Equations (24) and (25) provide estimates of the mass flow rate through vertical and horizontal two-dimensional sections in the model domain. By incorporating the above results into equation (18), air flow through the surfaces can be represented as a percentage of the total air flow out of the well.

SECTION 3.0--EVALUATION OF UNSATURATED ZONE AIR PERMEABILITY THROUGH PNEUMATIC TESTS

3.1 Overview of Pneumatic Pump Testing

Before proceeding to instructions for using AIR2D (Section 4), users unfamiliar with field methods for conducting pneumatic tests are advised to read this section. A knowledge of basic field data requirements and acquisition techniques makes it easier to understand the formatting of data input and output files as required and generated by AIR2D. Two procedures are presented for conducting pneumatic-pump tests to estimate the air-phase permeability in the unsaturated zone--the full-scale permeability test and the small-scale permeability test.

A full-scale permeability test is an in-situ procedure for determining the horizontal (k_r) and vertical (k_z) components of air permeability in the unsaturated zone. The procedure is directly analogous to the calibration method used in aquifer testing. The test procedure involves injecting or withdrawing air through a well screened in the unsaturated zone. The induced air flow stresses the domain, and the resulting pressure distribution, at steady state, can be measured by using a network of probes surrounding the well. Air-pressure measurements at the surrounding probes are made under static-flow conditions in the pipe that connects the probe to land surface with manometers or pressure transducers. The steady mass flow rate at the well also is measured. When the pressure at specific points in the domain and the air-flow rate are known, estimates for k_r, k_z, and if applicable, k' are obtained by calibrating the appropriate analytical solution with AIR2D. AIR2D executes the calibration procedure by using a least-squares parameter search. By refining the scale of the test, the air-permeability of small volumes of sediment can be determined. A major advantage of a full-scale test is that it provides estimates of air-permeability components k_r, k_z, and if applicable k', whereas a small-scale permeability test determines a single composite permeability. Full-scale tests, however, are costlier to implement.

The small-scale permeability test is intended to provide an air-permeability estimate for a small volume of sediment. Homogeneity ($k = k_r = k_z$) must be assumed because only one data point is available at the air withdrawal/injection location. The test procedure involves injecting or withdrawing air through a probe (screened well) located in the unsaturated zone. Pressure is measured at land surface by attaching a water manometer to the pipe connected to the probe. To determine the pressure at the probe, the surface pressure measurement is corrected for pressure losses due to air flow through the pipe (Section 3.3.1). Pressure losses can be significant for small-diameter pipes and high flow rates. The mass flow rate at steady state also must be measured. When the pressure at the probe and the mass flow rate are known, a composite estimate of air permeability ($k = k_r = k_z$) can be obtained by calibrating the air-flow models of AIR2D. The small-scale permeability technique is conceptually equivalent to performing a full-scale permeability test with a single pressure measurement in the domain. In the design of venting systems, an areal survey, consisting of several small-scale permeability tests, can be used to identify high permeability strata along which air will flow preferentially.

3.2 Full-Scale Permeability Field Tests

The equipment, procedures, and measurements that constitute the full-scale permeability tests are described in this section. The field data collected during the full-scale tests can be used to calibrate the analytical models that were discussed in Section 2.2 by using the computer program AIR2D.

3.2.1 Equipment and Measurements

A description of the equipment used at the Bemidji, Minn., and Galloway, N.J., research sites (Baehr and Hult, 1991; Fischer and others, 1991) is presented below. A schematic of the test equipment used at the Bemidji research site is shown in figure 4.

The full-scale permeability tests at both sites used wells constructed with stainless-steel casings and well screens. At the Bemidji site, casings had an inside diameter of 10.2 cm and a wall thickness of 0.64 cm. The well screen extended over a 60-cm interval. The well was set in a 23-cm-diameter hole drilled with a hollow-stem auger. The annulus between the casing and the borehole wall, adjacent to the screened intervals, was filled with pea gravel. To prevent airflow through the borehole annulus, a cement and bentonite grout was placed in the borehole interval from just above the screen to land surface.

At the Bemidji site, pressure probes were constructed from flexible copper tubing; the inside diameter of the tubing was 0.159 cm and the wall thickness was 0.159 cm. To form the probes, 10 cm of tubing was slotted at the lower end. The copper tubing extended to land surface and was attached to either a ± 5 lb/in^2 pressure transducer for digital recording of data or a water manometer for visual readings. The transducers used at the Bemidji and Galloway sites were manufactured by Setra Systems (model # 239) and Omega (model #PX170).

Probes surrounding the well were nested in holes drilled with a 10-cm-diameter auger at distances of 100, 300, and 1,000 cm from the center of the wells. The holes were filled with native sand, and granulated bentonite was used to provide a 10-cm-thick layer equidistant between vertically adjacent probes to prevent air flow in the annulus between probes. At Galloway, holes were drilled with a hand auger to obtain a detailed description of the sediment. Also clean sand was used between the bentonite seals because of simultaneous use of the holes for soil-gas surveys. Water manometers provided accurate measurements of steady-state air pressure at both sites, except for the pressure at the well screen of the pumped well where the water manometer readings attained impractically large values.

Thermistors (Yellow Springs Instruments, model #45016) were waterproofed and buried to determine the temperature profile in the unsaturated zone. The temperature, the probe depth below land surface (z), and the system pressure measured at the land surface (P_2) were used to adjust the probe pressure (P_1) according to the following relationship:

$$P_1 = P_2 \exp((\omega\ g\ z)/(R\ T_{ave})) \qquad (26)$$

where

T_{ave} = depth averaged temperature between probe and surface [Kelvin]

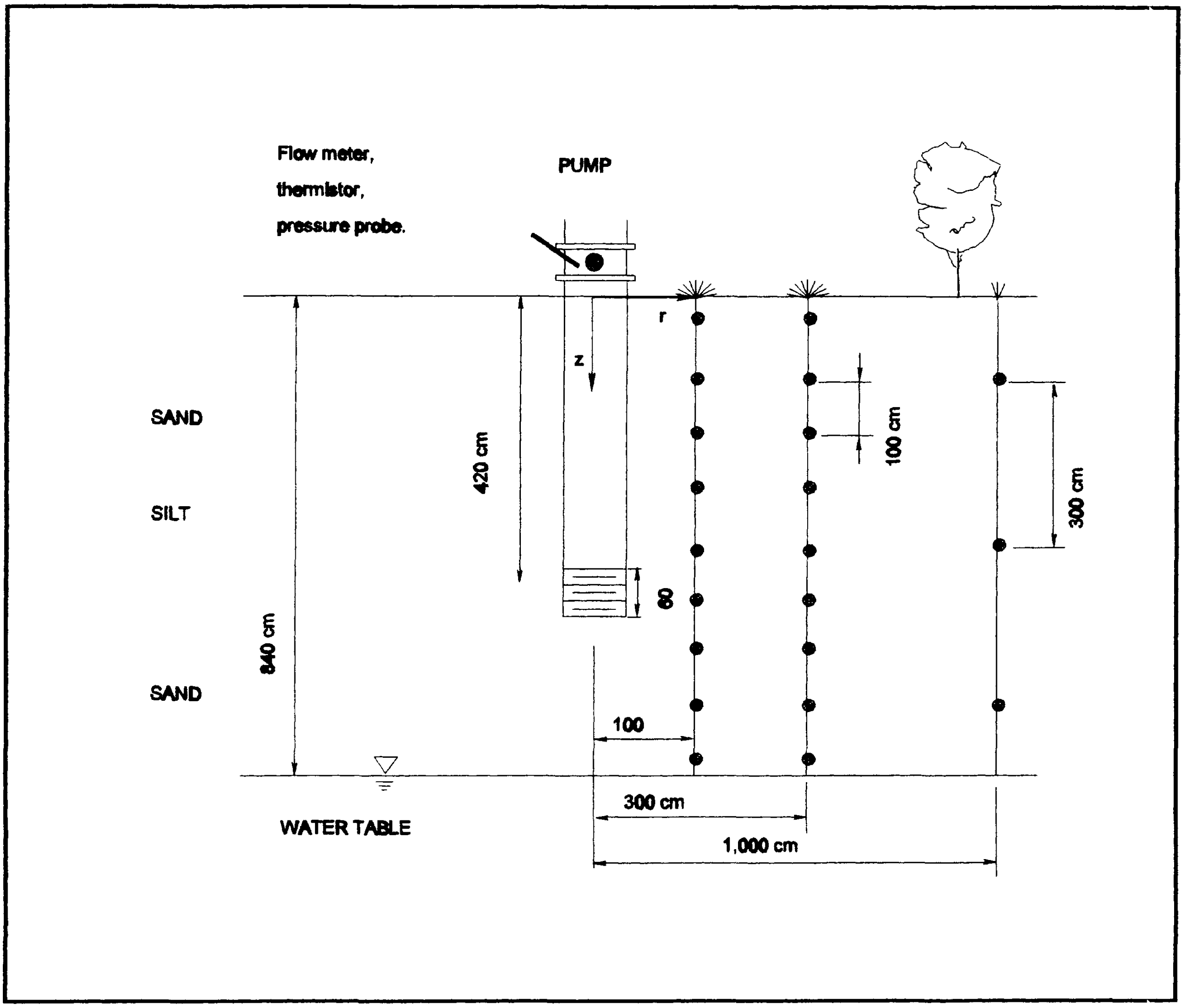

Figure 4.--Site instrumentation for conducting full-scale permeability tests at the Bemidji research site.

Results from the Bemidji site show that although the pressure adjustments made according to equation (31) were small, they fell within the range of instrument sensitivity. A thermistor and pressure probe were set in the well stand up to obtain the temperature and pressure of the air flowing out of and into the well. An Omega air flowmeter (model #FMA604V) was used to measure the velocity of air flow in the well: velocity, temperature, and pressure were used to obtain a mass flow rate. At Galloway, a Rotron regenerative blower (model # DR313) was used to induce flow.

Prior to beginning the test, atmospheric pressure and temperature are recorded. The test consists of injecting or withdrawing air through the well screened in the unsaturated zone. The pressure response throughout the monitoring network and the mass flux through the screen are measured during the test. Several different flow rates are used to obtain various flow versus pressure responses over a range of values. Only steady-state pressure readings can be used to calibrate AIR2D models. The steady-state condition is reached when the air flowmeter and water manometer or pressure transducers stabilize. Transient responses can be measured, however, when pressure transducers are used. The transient mass flow rate, determined with well instrumentation, is useful in identifying when steady-state conditions are achieved.

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3.2.2 Site Classification and Geology

Definition of the geology domain is based primarily on an interpretation of the boring logs made during the well and probe installation. As discussed previously, two models can be used to analyze the full-scale permeability test data. The first model applies to a domain open to the atmosphere (Section 2.2.1). The second applies to a domain separated from the atmosphere by a confining unit (Section 2.2.2). Choice of the model, and hence data collection requirements, depends on the geology of the site and the scale on which the testing is done. An important distinction in data collection for the two modeling alternatives is the location of the datum (or axes) used to measure depths. For an unconfined domain, depth measurements in the domain are made from the land surface. For a confined domain, depth measurements in the domain are made from the bottom of the upper unit. Therefore, the following geologic data are recorded

- presence or absence of an upper unit,
- thickness of upper unit,
- thickness of domain, namely distance between land surface (or bottom of upper unit) and the water table,
- depth to top of the sand pack around well screen from land surface or bottom of upper unit,
- depth to bottom of the sand pack around the well screen from land surface or bottom of upper unit.

3.3 Small-Scale Permeability Field Tests

During a small-scale permeability test, pressure is recorded only at the injection or withdrawal probe. Pressure along the pipe connecting the probe to the surface can drop significantly (for narrow pipes and high flow rates) compared with pressure drops that occur in the porous media. Hence, the loss in pressure must be taken into account when implementing the air-flow models. AIR2D accounts for pressure losses in pipes by incorporating equations from elementary fluid mechanics, as described in this section.

3.3.1 Pressure Loss Due to Flow Through a Pipe

For steady-state flow of a compressible fluid in a pipe, the equation that defines fluid pressure along the pipe is:

$$-\frac{dP}{dy} = \frac{f}{2D}\rho v^2 + \beta \rho v \frac{dv}{dy} \qquad (27)$$

where

P = pressure [g/cm-s^2]
y = coordinate along length of pipe [cm]
f = friction factor [-]
D = internal diameter of the pipe [cm]
ρ = density of the fluid (air) [g/cm^3]
v = velocity of fluid in pipe [cm/s]
β = constant (assumed to be unity here) [-]

Equation (27) incorporates the effects of friction and fluid compressibility. By substituting equations (4) and (6) into equation (27) and recognizing that $v\rho$ is constant for steady-state flow (that is, $v\rho = v_1 \rho_1$), the following expression is obtained,

$$-\frac{d\phi}{dy} = (v_1 \rho_1)^2 \frac{RT}{\omega}\left[\frac{f}{D} - \beta \frac{1}{\phi}\frac{d\phi}{dy}\right] \qquad (28)$$

where

ϕ = square of pressure [(g/cm-s^2)^2]
R = universal gas constant [g-cm^2/s^2-mol-K]
T = temperature of air in tube [K]
ω = average molecular weight of air phase [g/mol]
$v_1\rho_1$ = mass flow rate [g/cm^2-s]

Equation (28) is a non-linear ordinary differential equation that requires numerical solution. An approximate analytical solution to equation (28) is obtained by assuming that $(1/\phi)$ on the right hand side of the equation can be expressed as follows:

$$\frac{1}{\phi} \sim \frac{1}{\bar{\phi}} \qquad (29)$$

where

$$\bar{\phi} = P_1^2 \pm \left[(v_1 \cdot \rho_1)^2 \frac{RT}{\omega} \frac{f}{D} \right] \bar{y}$$

P_1 = system pressure measured at well head [g/cm-s^2]
v_1 = velocity of air in tube at P_1 [cm/s]
ρ_1 = density of the air in tube at P_1 [g/cm^3]
$\bar{y}$ = half the length of the tube [cm]
$+$ for withdrawal of air
$-$ for injection of air

The expression for $\bar{\phi}$ is obtained by neglecting the compressibility term $(\beta \rho v dv/dy)$ in equation (27). The solution obtained by substituting equation (29) into (27) agreed with a numerical solution to the original nonlinear equation. Therefore, the adjustment for pressure losses in the pipe incorporated into AIR2D is

$$\phi = P_1^2 \pm \left[\frac{C\,(f/D)}{C\,ß\,(1/\bar{\phi}\ ) - 1} \right] y \qquad (30)$$

where

$$C = (v_1 \cdot \rho_1)^2 \frac{RT}{\omega}$$

Equation (30) is used to predict pressure at the probe by using surface pressure measurements (P_1). All the factors needed to apply equation (30) can be measured directly with field equipment, except for the friction factor which must be obtained experimentally or from theoretical considerations. An overview of procedures that can be used to determine the friction factor is presented below.

3.3.2 Theoretical Evaluation of Friction Factors

Flow conditions in the well may be classified as laminar, transitional, or turbulent. The flow condition is defined by the Reynolds number:

$$Re = \frac{\rho \, v \, d}{\mu} \qquad (31)$$

where

Re = Reynolds number [-]
ρ = density of fluid [g/cm^3]
v = velocity of fluid [cm/s]
d = diameter of tube [cm]
μ = dynamic viscosity of fluid [g/cm-s]

On the basis of the Reynolds number, the following flow conditions can be identified.

$0 \leq Re \leq 2{,}000$ -> Laminar

$2{,}000 < Re < 4{,}000$ -> Transitional

$4{,}000 \leq Re$ -> Turbulent

Many theoretical formulations are available for predicting friction factors. The discussion here is limited to the equations used directly in the program AIR2D. Note, however, that the program also can accept friction factor input directly from the user. Thus, values based on any suitable method can be specified for the friction factor by the user. The equipment required to conduct the small-scale permeability analysis is sufficient to conduct experiments to determine the friction factor as a function of Reynolds number (see Section 3.3.3).

3.3.2.1 Theoretical Friction Factors for Laminar Flow Conditions

For laminar flow through a straight pipe of circular cross section, the following expression is used.

$$f = \frac{64}{Re} \qquad (32)$$

where

f = friction factor [-]
Re = Reynolds number ($Re < 2{,}000$) [-]

Equation (32) was developed from the Hagen-Poiseuille equations for flow through a pipe.

3.3.2.2 Theoretical Friction Factors for Turbulent Flow Conditions

Under turbulent flow conditions, the resistance to flow offered by the pipe walls depends to a large extent on the roughness of the wall surface. The wall roughness can be expressed in terms of a relative roughness term:

$$R_r = \frac{k}{D} \tag{33}$$

where

k = height of a surface protrusion [cm]
D = diameter of cross-section [cm]

When the roughness is minor, that is, all protrusions in the pipe wall can be contained within the laminar sublayer, the wall is considered to be hydraulically smooth. Then, the friction factor depends on the Reynolds number alone, and $R_r = 0$. When protrusions extend partly outside the laminar sublayer, additional resistance is encountered (compared with a smooth pipe) as a result of the protrusions in the boundary layer. Such sections are considered to be transition regions. In transition regions, the friction factor depends on the Reynolds number and on the relative roughness. When protrusions reach outside the laminar sublayer, by far the largest part of the resistance to flow results from the protrusions in the boundary layer. Such sections are considered to be completely rough regions. In completely rough regions, the friction factor depends on the relative roughness alone.

The above regions, described by Schlichting (1979), are incorporated in the Colebrook and White transition law (Colebrook and White, 1937). For turbulent flow through a straight pipe of circular cross section, the Colebrook and White transition law can be used to predict the friction factor as follows:

$$\frac{1}{(f)^{0.5}} = -2 \log \left(\frac{R_r}{3.7} + \frac{2.51}{(Re)(f)^{0.5}} \right) \tag{34}$$

where

f = friction factor of tube flow [-]
Re = Reynolds number (Re > 4,000) [-]

If the materials selected for use as connector pipes for probes are smooth (that is, $R_r = 0$), the need to evaluate R_r is eliminated.

3.3.2.3 Theoretical Friction Factors for Transitional Flow Conditions

A transition region is present for the Reynolds numbers from about 2,000 to 4,000, the range in which flow changes from laminar to turbulent conditions. In the transition region, flow is inherently unstable, and expressions for evaluating friction factors are generally inaccurate. AIF 2D obtains theoretical friction factors in the transition region by linearly interpolating between friction factor values at Reynolds numbers of 2,000 and 4,000.

3.3.2.4 Minor Friction Losses in Tubes

Note that the equations used to predict friction factors apply only to fully developed flow. When a fluid enters a circular pipe, the velocity distribution across the pipe varies with the distance from the inlet (Schlichting, 1979). The velocity distribution is nearly uniform near the inlet. Farther downstream the velocity distribution changes as a result of the influence of friction, until a fully developed velocity profile is attained at a distance L_i from the inlet and remains constant downstream so that

$$L_i = (0.03)(D)(Re) \quad \text{for laminar flow} \qquad (35)$$

$$25(D) < L_i < 100(D) \quad \text{for turbulent flow} \qquad (36)$$

where

D = internal tube diameter [cm]

Re = Reynolds number [-]

A simplifying assumption made in the small-scale permeability analysis is that friction losses over the entire length of the pipe can be approximated by losses associated with fully developed flow. Ideally, the user should ensure that this assumption is valid under the test conditions being investigated. A second simplifying assumption is that the losses arising from changes of section, junctions, bends, and valves are considered negligible. The program AIR2D does not provide for any means of incorporating these losses into the analysis.

The minor friction losses in the pipes, the assigned values for the relative roughness terms, and the implicit assumptions incorporated in the theoretical approach introduce a level of uncertainty in the friction-factor predictions. A more reliable approach to quantifying friction losses in the probe pipe is the use of experimental techniques. The experimental approach is presented in the next section. In general, the model sensitivity to friction factor selection is significant. Ideally, the user should always test the effect of friction-factor selection on the model output.

3.3.3 Experimental Evaluation of Friction Factors

Friction factors also can be obtained by using experimental data to calibrate equations that describe friction losses. The field procedure involves withdrawing air through a length of tubing and measuring the pressure drop between the ends. One end of the tube remains at atmospheric pressure during the experiment. A manometer and flowmeter are connected to the other end of the tube. By varying air flow through the tube section, pressure drops can be measured over a range of flow rates. By rearranging the pipe-flow solution given by equation (35), an estimate for the friction factor is obtained as follows:

$$f = \frac{D}{L}\left[\frac{\beta}{\Phi} - \frac{\omega}{RT}\frac{1}{(v_1\,\rho_1)^2}\right]\left[P_1^2 - P_{atm}^2\right] \qquad (37)$$

where

$$\Phi = \frac{1}{2}\left[P_1^2 + P_{atm}^2\right]$$

L = tube length [cm]

β = constant (assumed to be unity) [-]

The Reynolds number, corresponding to the flow conditions at which the friction factor was determined, can be calculated by using equation (31). Hence, a series of Reynolds number-friction factor correlations can be generated for different flow rates. Interpolation is necessary to estimate friction factors for the test measurements over a continuum of Reynolds numbers. A cubic spline technique (Gerald and Wheatley, 1989) is included in AIR2D to perform this task. AIR2D uses a cubic spline to interpolate data sets containing discrete Reynolds number-friction factor correlations, thereby predicting intermediate values. Hence, experimental friction-factor data can be used in actual test simulations in which a wide range of Reynolds numbers are encountered.

3.3.4 Equipment and Measurements

Basic components of the field equipment necessary to perform the small-scale permeability evaluations of the unsaturated zone include

- a length of pipe with a probe at the end,
- a water manometer or pressure transducer,
- a flowmeter (for example, a rotometer),
- a chamber to trap water,
- a pneumatic pump (and power supply),
- a thermometer or thermistor, and
- a barometer for determining prevailing atmospheric pressure.

A brief description of the technique as applied at the Galloway research site (Joss and others, 1991) is presented below. Figure 5 is a schematic of the test equipment as it is setup at the site.

At the Galloway site, probes used for small-scale permeability tests also were used for unsaturated zone vapor sampling; therefore, narrow (0.25-inch diameter) stainless-steel tubing was used to fashion the probes, that were open at land surface. Ideally, wider tubing is used for a small-scale permeability test to minimize pressure loss at high air-flow rates. Vapor probes at the site were located at the midpoints of lithologic units in the unsaturated zone. Probes were set in hand-augured boreholes about 7.6 cm in diameter. The annulus between the probe and the borehole wall was filled with a coarse silica sand. The sand pack surrounding each probe was sealed at top and bottom with bentonite to prevent air movement along the borehole. Because of the high permeability of the sand pack relative to the in situ material, the pressure drop between the probe and the borehole wall was assumed to be negligible. This assumption required that the dimensions of the sand pack, rather than the tube diameter, be used as the well radius in AIR2D. Similarly, the length of the sand pack, rather than the length of the slotted interval at the tube end forming the probe, was assumed to be the well-screen length. Under moist conditions, the test can induce water movement in the unsaturated zone that can flow through the system and foul the flowmeter. A water trapping chamber was installed between the water manometer and the flowmeter to capture any water entering the system (see figure 5).

Rotometers were used to measure air-flow rates ranging from 0 through 80 liters per minute. The following rotometers were used at the Galloway site:

- Gilmont (serial no. E9382), size 5, with glass float (BB);
- Cole-Parmer (flowmeter serial no. 006211) (tube serial no. N034-39), with stainless steel float (ST);
- Cole-Parmer (tube serial no. N082-03) with stainless steel float (ST).

The following rotameter adjustment formula from Perry and Green (1984) compensates for the effects of nonstandard temperatures and pressures on flow-rate measurements.

$$q_a = \left[\frac{P_b\,T_a}{P_a\,T_b}\right]\left[\frac{P_a\,T_b}{P_b\,T_a}\right]^{1/2} q_b \qquad (38)$$

where

q_a = corrected flow rate for prevailing P_a and T_a [cm^3/s]

q_b = actual flow rate for standard P_b and T_b [cm^3/s]

P = pressure [$g/cm\text{-}s^2$]

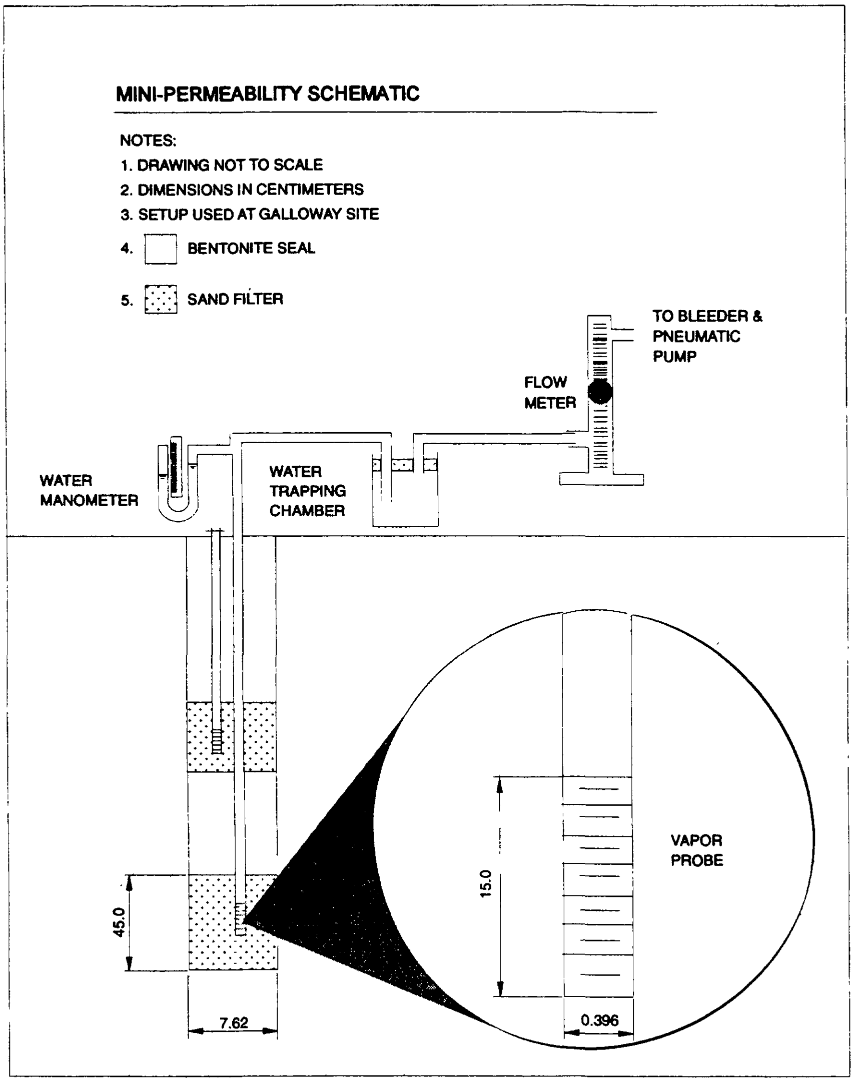
T = temperature [K]

The pump and motor used at the Galloway site were as follows:

- Gast Manufacturing, Inc. Pump (model number 0522-V4FG180DX, serial number 0689);
- Emmerson 1/3 horsepower Motor, 1,725 revolutions per minute (model number SA 55NXGTC-4143).

At Galloway, as previously mentioned, the vapor probes were installed by using a 7.6-cm hand auger; therefore, it was possible to document the stratigraphy on the scale of inches. If mechanical drilling techniques are used, ideally split-spoon sampling should be performed to characterize the lithology of the unsaturated zone. Probe depths were selected to coincide with the mid-point of each unit. Because one borehole typically intersected several lithologic units, probes were nested in the boreholes. Near the surface, a PVC riser pipe was installed in the borehole and protruded a short distance above the land surface. A cap on the riser pipe provided additional protection for the tubing attached to the probes.

Flexible tubing connected the probe and steel tubing at the surface to the pump and measuring devices. Prior to beginning the test, atmospheric pressure and temperature were recorded. This information is needed to correct rotometers for non-standard flow conditions. The pneumatic pump was then turned on and adjusted to give the desired air-flow rate through the vapor probe; ideally, tests should be performed over a range of flow rates. Results obtained from the Galloway site suggest that the data become more representative of field conditions as the flow rate increases. This could result because air-permeability values are averaged over larger geologic areas, and thus, tend to control variations. The system should be allowed to reach steady state prior to taking any measurements. Bentonite seals between vertically adjacent probes can be tested by pumping one probe and measuring the pressure in the other. If seals are intact and if the vertically adjacent probes are in the dead zone of the induced flow field, no pressure change is recorded.



NOT TO SCALE

Figure 5. Site instrumentation for conducting small-scale permeability tests at the Galloway, New Jersey, research site.

SECTION 4.0--AIR2D, A COMPUTER PROGRAM TO SIMULATE TWO-DIMENSIONAL AXISYMMETRIC AIR FLOW IN THE UNSATURATED ZONE

AIR2D is the computer program that implements the air-flow model described in Section 2.0. The program can be used in a calibration mode to analyze the results of pneumatic tests (see Section 3.0) or in a prediction mode to quantify pressure and flow distribution in the domain at specified locations.

In order to use AIR2D, data files containing geologic, well, air-flow rate, and pressure data must be set up. AIR2D provides editing options for creating and modifying the data input files. Alternatively, system editing programs can be used to set up the appropriate files. Details of the file layout and contents are presented in the following sections. Output from AIR2D can be directed to the screen or to output files.

AIR2D uses a modular structure that enables the modification of subroutines to be performed with relative ease. The program is written in Fortran 77 and, with minor changes, should run on a variety of computer systems, including mainframes and personal computers.

4.1 Basic Operations

This Section outlines modifications to the code, compilation procedures, and data entry requirements necessary to run AIR2D.

4.1.1 Getting Started

The source code AIR2D.FOR (on personal computers) or AIR2D.F77 (on mainframes) should be loaded into an editing package on the computer system and checked for compatibility with the operating environment.

For operation on a mainframe computer, the code in the main calling program should appear as follows:

```
C
C4----ASSIGN BASIC INPUT UNIT AND PRINTER UNIT.
C    SET: INBAS = 5  WHEN USING PERSONAL COMPUTER
C    SET: INBAS = 1  WHEN USING MAINFRAME
C    SET: IOUT  = 6  WHEN USING PERSONAL COMPUTER
C    SET: IOUT  = 1  WHEN USING MAINFRAME
C
   INBAS=1
   IOUT=1
C
```

For operation on a personal computer, the code in the main calling program should appear as follows:

```
C4----ASSIGN BASIC INPUT UNIT AND PRINTER UNIT.
C    SET: INBAS = 5  WHEN USING PERSONAL COMPUTER
C    SET: INBAS = 1  WHEN USING MAINFRAME
C    SET: IOUT  = 6  WHEN USING PERSONAL COMPUTER
C    SET: IOUT  = 1  WHEN USING MAINFRAME
C
     INBAS=5
     IOUT=6
```

The program performs calculations in double precision. This could be burdensome for small computer systems. The following statement can be removed from each subroutine in the program to calculate in single precision:

```
     IMPLICIT DOUBLE PRECISION(A-H,O-Z)
```

In addition, functions such as DABS, DSQRT, DSIN, DCOS, DTAN, DBSK1, DBSK0, and others must be changed to ABS, SQRT, SIN, COS, TAN, BSK1, BSK0, and so on.

The solutions to the air-flow equation require evaluation of $K_0(x)$ and $K_1(x)$, the zero and first-order modified Bessel functions of the second kind, respectively. AIR2D invokes FUNCTIONs within the program to evaluate these Bessel functions, when required. An alternate method of evaluating the Bessel functions is to use commercially available software programs such as the IMSL math libraries. These mathematical libraries can replace the programmed Bessel FUNCTIONs. The procedure involves deleting the following Bessel FUNCTIONs from AIR2D:

```
     FUNCTION DBSK0(X)
     FUNCTION DBSK1(X)
```

The user then makes use of the external functions by ensuring the Bessel FUNCTION names in AIR2D (for example DBSK0(x) and DBSK1(x)) correspond to those in the package being used. If not, the FUNCTION names in AIR2D must be changed to match those of the external program. Then AIR2D is compiled and linked to the external mathematics library. This procedure allows AIR2D to use external software.

In certain instances, selected arrays in AIR2D may need to be redimensioned. For example, in the subroutine FRIKF, the number of points used to perform cubic spline interpolations should not exceed 50. When additional points are available, XV(LENX) should be redimensioned by changing the value assigned to LENM in the PARAMETER statement in the main program. Similarly, in the subroutine POWELL, the number of pressure observations that can be used to calibrate the air-flow models cannot exceed 100 without redefining LENP in the PARAMETER statement in the main program. Additional unit systems can also be added to the program by incorporating the necessary information in the subroutines SETUP, DATAIN, and POWELL, and modifying LENU in the PARAMETER statement in the main program. The lines requiring modification in the main program are shown below:

```
PARAMETER(LENM=50,LENP=100,LENU=7,LENS=10)
COMMON XV(12*LENM),RD(LENP),ZDA(LENP),PHID(LENP)
COMMON XSTOR(23*LENS),ASTORA(LENS)
COMMON IU1(LENU),XU2(LENU,10),IU3(LENU,10)
```

Whenever modifications or changes are made to the program source code, the program must be recompiled so that the alterations are incorporated into the executable version of the program code. The program is written in Fortran 77. Thus, any standard Fortran 77 compiler can be used to recompile the code. Commands needed to compile AIR2D on a personal computer depend upon the system and type of compiler used. The following command compiles and links the program on an IBM personal computer using Microsoft's Fortran compiler:

```
FL AIR2D.FOR
```

To execute the program on a personal computer, change to the directory containing the program executable code (for example, AIR2D.EXE created in the above compilations step), and at the prompt, type in:

```
AIR2D
```

An introductory screen appears, prompting the user to select the application.

4.1.2 Data Input Files

After invoking the program, the following menu with options will appear on the screen:

```
          AIR2D (Version 3.1)

          by  CRAIG JOSS
              ARTHUR BAEHR

   SELECT:

   1. TO RUN AIR2D BY USING AN EXISTING DATA FILE
   2. TO MODIFY AN EXISTING DATA FILE
   3. TO CREATE A NEW DATA FILE
   4. TO END PROGRAM

   PLEASE SELECT NUMBER  1, 2, 3  OR  4:
```

To implement AIR2D, data must be entered from input files. For Option 1, more than one data file may be required, depending on the particular program application. The files required for each application, their contents, and formats are described in Sections 4.2 through 4.5. Error trapping routines in AIR2D check for file presence and completeness. The program tests for END OF FILE input errors. When the information in the data files is incomplete, the program will display an error message indicating that an unexpected END OF FILE was encountered. In most instances, the program will identify the file in which the data-entry error occurred. The program then will terminate, allowing the data error to be corrected in the particular data file.

The names of the input data files are determined by the user. This provides flexibility in data selection when multiple runs are performed. Note, however, that certain system limitations exist regarding the length of filenames and the types of characters that can be used.

In general, all files used for the entry of data should be located in the same directory as the executable program file. With certain computer systems, such as personal computers, the data files can be accessed from subdirectories, providing that the full path is specified in the filename. For applications of AIR2D, the executable version of the program code is required, as well as input data files as follows:

·	AIR2D.SEG	(executable code for mainframe computers) or
·	AIR2D.EXE	(executable code for personal computers),
·	TESTxxx	(data file required for all program applications),
·	CALIBxxx	(data file required only when flow rates are specified in terms of scale readings), and
·	FRICxxx	(data file required only for small-scale permeability applications).

If Option 2 (modify existing file) or Option 3 (create a new file) is selected, a series of prompts requesting input of the data needed for the data files will appear on the screen. For Option 2, the user must specify the name of the file containing the information to be modified. AIR2D reads in the data contained in the specified file and displays it as examples accompanying the input prompts (indicated by EG). If no change is to be made to the example value, the user presses the ENTER or CARRIAGE RETURN key to accept the value. Alternatively, if the user specifies a new value, the example value will be overwritten. Note that for a few cases (indicated by EG* in the prompts), the user must input the default value and cannot use the ENTER feature described above. For Option 3, the user must specify each entry. Examples accompanying the prompts are for illustration purposes only and will not be recorded by pressing ENTER. The precise nature of information required to set up the data files will be determined by the type of application. After the necessary data have been entered, the information is written to formatted data files for use in AIR2D. Option 1 allows the user to bypass the AIR2D input file editor because input file(s) can be created by using a system text editor, if the file layout and contents correspond to the formats discussed in Sections 4.2 through 4.5.

4.1.3 AIR2D Applications

If the user runs AIR2D with an existing file, a menu with four options will appear on the screen as shown below:

```
AIR2D APPLICATION MENU

SELECT:

1. TO ANALYZE FULL-SCALE PERMEABILITY DATA
2. TO ANALYZE SMALL-SCALE PERMEABILITY DATA
3. TO EVALUATE PIPE FRICTION FACTOR
4. TO PREDICT PRESSURE AND FLOW IN DOMAIN

PLEASE SELECT NUMBER 1, 2, 3,  OR  4:
```

Option 1 provides a method for analyzing full-scale pneumatic-pump test data to obtain horizontal (k_r) and vertical (k_z) air-phase-permeability estimates for the domain, and if applicable, the air-phase permeability (k') of a upper lithologic unit. Section 4.2 presents the input and output requirements associated with Option 1.

Option 2 provides a method for analyzing small-scale pneumatic pump test data to obtain composite (k) air-phase-permeability estimates. Section 4.3 presents the input and output requirements associated with Option 2. In order to perform the small-scale permeability analysis, estimates of the friction factor governing air flow in the pipe are required. Option 3 provides a method for evaluating the friction factor from experimental tests. Alternatively, the friction factor can be evaluated from theoretical formulations by using either Option 2 or 3.

Option 4 is used to predict pressure and air flow in the unsaturated zone for an assumed air-permeability distribution. Because transport of contaminants in the vapor phase depends directly on the air-flow rates, output from Option 4 can be used in the design of soil venting systems. In summary, Options 1 through 3 are used to solve calibration problems, and Option 4 is used to make predictions.

Depending on the type of application, the processing time needed to perform a simulation can take from a few seconds to several hours. When performing friction-factor evaluations (Option 3) and pressure and flow predictions (Option 4), the processing time is on the order of seconds. Note that, AIR2D may terminate prematurely if the values generated for flows are physically unattainable. When performing permeability calibrations (Options 1 and 2), the processing time is sensitive to input data. Probably the most significant factor influencing the time needed for program execution is the order of the parameter search increment (DINC) and decrement (DECR) used in the hill descending algorithm (see Sections 4.2.1 and 4.3.1). When refined searches are specified (for example DINC = 1.0001 and DECR = 0.9999), processing time can be several hours. Ideally, on the first application of the program, the user should select a coarse value for the search parameters (for example, DINC=1.01 and DECR=0.99). Permeability estimates generated by the initial simulation then can be used in subsequent simulations as the estimated values required for the input files. These initial estimates for permeability narrow the search; therefore the computation times associated with crude initial estimates are not excessive.

4.1.4 Data Categories, Units, and Default Settings

The data required to implement the program AIR2D fall into four categories--default settings, experimental measurements or operational conditions, program control data, and correlation data.

1. Default Settings

Default settings include

- PI = 3.14159 [Constant]
  [Dimensionless]
- BETA = 1.0 [Constant ß in pipe-flow equation (32)]
  [Dimensionless]
- VAS = 0.000176 [Viscosity of air at TVAS]
  [Units in g/cm-s]
- TVAS = 293.15 [Temperature at which VAS applies]
  [Units in K]
- RG = 83140000.0 [Universal gas constant]
  [Units in g-cm^2/s^2-mol-K]
- WAIR = 28.8 [Average molecular weight of air]
  [Units in g/mol]
- STDATM = 1013250.0 [Pressure conversion from atmosphere to metric units]
  [Units in g/cm-s^2].

Default settings should remain constant.

The conversion factors listed below are included in the subroutine SETUP to enable the user to input data and review output in a specified unit system. Options include

- length units, where
  1 cm = 1.0 x 10^{-1} dm = 1.0 x 10^{-2} m = 3.937 x 10^{-1} in
  = 3.281 x 10^{-2} ft = 1.0937 x 10^{-2} yd

- volume units, where
  $1\ cm^3 = 1.0 \times 10^{-3}\ L = 1.0 \times 10^{-6}\ m^3 = 6.1023 \times 10^{-2}\ in^3$
  $= 3.5314 \times 10^{-5}\ ft^3 = 1.3079 \times 10^{-6}\ yd^3 = 2.6417 \times 10^{-4}\ gal$

- time units, where
  $1\ s = 1.6667 \times 10^{-2}\ min = 2.7778 \times 10^{-4}\ hr$
  $= 1.1574 \times 10^{-5}\ d = 3.1688 \times 10^{-8}\ yr$

- pressure units, where
  $1\ atm = 760\ mm\text{-}Hg = 406.38\ in\text{-}H_2O = 101.325\ kPa = 14.70\ lb/in^2$

- temperature units, where
  $t_c\ °C = t_k - 273.15\ K = (t_f - 32) / 1.8\ °F$

- mass units, where
  $1\ g = 1.0 \times 10^{-3}\ kg = 2.2046 \times 10^{-3}\ lb$

- permeability units, where
  $1\ cm^2 = 1.0 \times 10^{-2}\ dm^2 = 1.0 \times 10^{-4}\ m^2 = 1.550 \times 10^{-1}\ in^2$
  $= 1.076 \times 10^{-3}\ ft^2 = 1.1962 \times 10^{-4}\ yd^2 = 1.0 \times 10^{8}\ darcy.$

The user can select any combination of unit systems. If no unit system is specified, AIR2D defaults to the first unit system in the above list.

2. Experimental Measurements or Operational Conditions

In this input category, either experimental measurements for calibration applications or operational conditions for prediction applications, comprise the data set. Input includes factors such as:

- project location,
- test date,
- equipment information,
- definition of site geology,
- air-flow rates,
- pressure measurements, and
- prevailing temperature and pressure conditions.

The data set will change from simulation to simulation and, therefore, must be entered for each program application.

3. Program Control Data

The third category of data input is program control data. This information controls the program by directing and (or) limiting the program operations. A partial list of program operations that can be controlled by this data set includes

- maximum number of iterations,
- closure criteria,
- decrements and increments used to modify permeability estimates,
- number of sets of input data, and
- input/output filenames.

Program control data must be specified for each simulation.

4. Correlation Data

Sets of correlation data are used to convert raw test data into forms that are suitable for use in the model solutions. For example, flowmeter scale readings as they relate to standard flow rates can be input to perform required interpolation. If test data are in forms suitable for use in the model, no correlation data are required.

4.1.5 Output Files

AIR2D output depends on the particular application. In the calibration mode, permeability estimates, corresponding to various air-flow rates, are tabulated along with the prevailing pressure and temperature and a summary of the input data. Output for Options 1, 2, and 3 is written to the screen and, if specified by the user, is output to a file. Output filenames may be specified in the input file or interactively from the screen.

In the prediction mode, pressure and air-flow output are written to separate output files. If no output names are specified, the program assigns the following output filenames for Option 4 simulations:

PVSR.OUT	for pressure predictions,
VVSR.OUT	for volumetric flow predictions,
MVSR.OUT	for mass flow predictions, and
WELL.OUT	for pressure, volumetric flow and mass flow at the well.

WELL.OUT also records the unit system used in the simulation. Note that care is exercised when selecting output filenames because information in existing files will be overwritten with each simulation.

4.2 AIR2D - Application to Determine Air-Phase Permeability with a Full-Scale Permeability Test

To solve the air-permeability-calibration problem by using AIR2D to analyze data from a full-scale test (see Section 3.1), the following data files are used

1) TEST1xx - TEST1xx is used to input field data and program control information (Section 4.2.1),

2) CALIBxx - CALIBxx is used to input correlations between flowmeter scale readings and flow rates in specified unit systems under standard conditions (Section 4.2.2).

The file TEST1xx is required for full-scale permeability applications. CALIBxx is usually optional; it is required only when flow rates are input in terms of flowmeter scale readings. If flow rates entered in TEST1xx can be used directly in the air-flow models, CALIBxx can be omitted. The user can specify the unit system to be used for length, volume, time, pressure, temperature, mass, and permeability data. Output from full-scale permeability simulations is always displayed on the screen. The user can specify that the output be written to a file. This can be done interactively or by direct entry using the data input files. Section 4.2.3 presents an example of the full-scale output.

4.2.1 Input File TEST1XX

TEST1XX specifications are as follows:

Name of file:	Specified by the user after invoking AIR2D.
File contents:	Project, date, well number, direction of air flow, output filename, number of flow measurements, geologic characteristics/model selection, units, number of iterations, closure criteria, properties of the upper unit, properties of the domain, model decrements or increments, well or domain dimensions, prevailing conditions, and flow and pressure-test measurements.
File application:	This file inputs data from full-scale tests, which are used to evaluate air permeability. This file is required for all full-scale permeability applications.
File unit number:	The program defines the TEST1xx input file as UNIT = 8.
Program input:	Data from the TEST1xx file is input to three subroutines. General test details are accessed from the subroutine SETUP once per simulation. Flow and pressure measurements are accessed from the subroutine DATAIN several times per simulation, depending on the number of variations in flow rates (NR). Pressure response measurements in the domain are input to the subroutine POWELL several times per simulation, depending on the number of monitoring points (NPTS).
Data units:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output can be specified by the user. If no unit system is specified, units must conform to the default unit systems for each data value.

The structure and formatting of the TEST1xx input file are shown below. Variables are defined following the example of the file.

1. Data: PROJECT
   Format: A40

2. Data: DATE
   Format: A12

3. Data: WELLNUM
   Format: A12

4. Data: DINJ,AOUT
   Format: F10.6,A12

5. Data: NR,IOP1,IOP2,IU1(1),IU1(2),IU1(3),IU1(4),IU1(5),IU1(6),IU1(7)
   Format: 10I5

6. Data: NMAX,RER
   Format: I10,E10.3

IF IOP2 = 2 (ie. upper unit of lower permeability present) THEN
INPUT Item 7 ELSE LEAVE BLANK LINE IF IOP2 = 1

7. Data: B1,XK1
   Format: F10.3,E10.3

8. Data: AR,XKR
   Format: F10.3,E10.3

9. Data: DECR,DINC
   Format: 2F10.4

10. Data: ZD,ZL,ZB,RW
    Format: 4F10.3

INPUT Items 11 and 12 NR TIMES (i.e. once for each test)

11. Data: NPTS,TAIR,TSOIL,ATM,P3,Q4,AFLOW
    Format: I2,F8.3,4F10.3,A12

INPUT Item 12 NPTS TIMES (i.e. once for each probe measurement)

12. Data: RD(I),ZDA(I),PHID(I)
    Format: 2F10.3,F10.5

An example of TEST1XX is shown below.

```
                                                  Input records
Data    Explanation                     |---+----+----+----+----+----+----+----+----+----+
item                                    1   5   10   15   20   25   30   35   40   45   50
 1.PROJECT------------------------------FULL SCALE PERMEABILITY TEST - RIGOROUS
 2.DATE---------------------------------06/04/1991
 3.WELLNUM-----------------------------  9
 4.DINJ,AOUT--------------------------- -1.0     TESTFULL.OUT
 5.NR,IOP1,IOP2,IU1(1),.,IU1(7)--------     3    2    2    1    1    1    1    1    1    1
 6.NMAX,RER----------------------------   10000000 1.000E-05
 7.B1,XK1------------------------------     10.000 5.000E-09
 8.AR,XKR------------------------------      1.200 5.000E-08
 9.DECR,DINC---------------------------     0.9900    1.0100
10.ZD,ZL,ZB,RW-------------------------     27.000    58.000   118.000     3.800
11.NPTS,TAIR,TSOIL,ATM,P3,Q4,AFLOW-(1)- 3  22.000    17.000     0.992     0.874      39.00 CALIBGM1.CPS
12.RD(I),ZDA(I),PHID(I)--(PROBE 1)-----      3.810    42.500   0.97731
12.RD(I),ZDA(I),PHID(I)--(PROBE 2)-----     50.000     1.000   0.99124
12.RD(I),ZDA(I),PHID(I)--(PROBE 3)-----     50.000    67.000   0.99129
11.NPTS,TAIR,TSOIL,ATM,P3,Q4,AFLOW-(2)- 3  22.000    17.000     0.992     0.916      29.00 CALIBGM1.CPS
12.RD(I),ZDA(I),PHID(I)--(PROBE 1)-----      3.810    42.500   0.97734
12.RD(I),ZDA(I),PHID(I)--(PROBE 3)-----     50.000     1.000   0.99149
12.RD(I),ZDA(I),PHID(I)--(PROBE 3)-----     50.000    67.000   0.99151
11.NPTS,TAIR,TSOIL,ATM,P3,Q4,AFLOW-(3)- 3  22.000    17.000     0.992     0.963      16.00 CALIBGM1.CPS
12.RD(I),ZDA(I),PHID(I)--(PROBE 1)-----      3.810    42.500   0.98512
12.RD(I),ZDA(I),PHID(I)--(PROBE 2)-----     50.000     1.000   0.99171
12.RD(I),ZDA(I),PHID(I)--(PROBE 3)-----     50.000    67.000   0.99166
```

Definitions of input variables in the TEST1xx file are presented below. The user can select the most convenient unit systems for input/output of data. If no unit systems are specified, units must conform to the default unit systems. Variables are presented in the same order as they appear in the data input file.

PROJECT:

- PROJECT is the project title or description identifying test data.
- PROJECT is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to PROJECT, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 40 characters: (A40).
- Input example: FULL-SCALE PERMEABILITY TEST.

DATE:

- DATE is the date of the full-scale-permeability field test.
- DATE is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to DATE, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: 06/04/1991.

WELLNUM:

- WELLNUM is the identification number assigned to the well used in the field test.
- WELLNUM is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to WELLNUM, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: 9.

DINJ:

- DINJ is the variable that records whether air was withdrawn (DINJ=-1.0) or injected (DINJ=1.0) during the full-scale permeability test.
- DINJ must be specified in order to implement the air-flow model. If the absolute value of DINJ does not equal 1.0, an error message will be displayed.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: -1.0 (for air withdrawal),
  1.0 (for air injection).

AOUT:

- AOUT is the name of the output file that records permeability evaluations.
- AOUT is optional. If AOUT is not specified, the program will prompt the user to specify whether output should be displayed on the screen or written to a data file. If the user selects a data file for output, the program prompts the user for the name of the output file. If no name is assigned to AOUT, the output will be displayed on the screen and not saved.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: TESTFULL.OUT.

NR:

- NR is the number of variations in well injection/withdrawal air-flow rates for which pressure measurements in the domain were obtained. For a single application of AIR2D, NR cannot exceed 10.
- NR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 3.

IOP1:

- IOP1 is the variable that records whether domain is isotropic, $k_r \approx k_z$ (IOP1 = 1), or anisotropic, $k_r \neq k_z$ (IOP1 = 2).
- If IOP1 is not specified, the program will default to the setting IOP1=1, an isotropic domain.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1 for isotropic domain,
  2 for anisotropic domain.

IOP2:

- IOP2 records whether an upper unit of low permeability (between the well and the atmosphere) is absent (IOP2 = 1) or present (IOP2 = 2). The selection of IOP2 determines the analytical solution used in the program AIR2D. For IOP2 = 1, the solution presented in Section 2.3.1 is used. For IOP2=2, the solution presented in Section 2.3.2 is used.
- IOP2 defaults to a value of 1 (no upper unit present and domain open to atmosphere) when no value is specified by the user.

- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 2.

IU1(1):

- IU1(1) is the specification for input and output of length units, where

  IU1(1) = 0 or 1 for length in units of centimeters (cm),
  IU1(1) = 2 for length in units of decimeters (dm),
  IU1(1) = 3 for length in units of meters (m),
  IU1(1) = 4 for length in units of inches (in.),
  IU1(1) = 5 for length in units of feet (ft), and
  IU1(1) = 6 for length in units of yards (yd).

  Note: 1 cm = 1.0×10^{-1} dm = 1.0×10^{-2} m = 3.937×10^{-1} in.
  = 3.281×10^{-2} ft = 1.0937×10^{-2} yd.

  The unit system selected applies to all length units in the input and output data files.
- IU1(1) defaults to a value of 1 (length units in centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(2):

- IU1(2) is the specification for input and output of volume units, where

  IU1(2) = 0 or 1 for volume in units of cubic centimeters (cm^3),
  IU1(2) = 2 for volume in units of liters (L),
  IU1(2) = 3 for volume in units of cubic meters (m^3),
  IU1(2) = 4 for volume in units of cubic inches ($in.^3$),
  IU1(2) = 5 for volume in units of cubic feet (ft^3),
  IU1(2) = 6 for volume in units of cubic yards (yd^3), and
  IU1(2) = 7 for volume in units of gallons (gal).

  Note: 1 cm^3 = 1.0×10^{-3} L = 1.0×10^{-6} m^3 = 6.1023×10^{-2} in^3
  = 3.5314×10^{-5} ft^3 = 1.3079×10^{-6} yd^3 = 2.6417×10^{-4} gal

  The unit system selected applies to all volume units in the input and output data files. Note that the volumetric unit system does not have to correspond to the length unit system.
- IU1(2) defaults to a value of 1 (volume units in cubic centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(3):

- IU1(3) is the specification for input and output of time units, where

  IU1(3) = 0 or 1 for time in units of seconds (s),
  IU1(3) = 2 for time in units of minutes (min),
  IU1(3) = 3 for time in units of hours (hr),
  IU1(3) = 4 for time in units of days (d), and
  IU1(3) = 5 for time in units of years (yr).

  Note: 1 s = 1.6667×10^{-2} min = 2.7778×10^{-4} hr
  = 1.1574×10^{-5} d = 3.1688×10^{-8} yr

  The unit system selected applies to all time units in the input and output data files. Hence, for the above selections, the corresponding volumetric or mass-flow-rate output units are flow per second, flow per minute, flow per hour, flow per day, or flow per year, respectively.
- IU1(3) defaults to a value of 1 (time units in seconds) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(4):

- IU1(4) is the specification for input and output of pressure units, where

  IU1(4) = 0 or 1 for pressure in units of atmospheres (atm),
  IU1(4) = 2 for pressure in units of millimeters of mercury (mm-Hg),
  IU1(4) = 3 for pressure in units of inches of water (in-H_2O),
  IU1(4) = 4 for pressure in units of kilopascals (kPa), and
  IU1(4) = 5 for pressure in units of pound per square inch (lb/in^2).

  Note: 1 atm = 760 mm-Hg = 406.38 in. of H_2O = 101.325 kPa = 14.70 lb/in^2

  The unit system selected applies to all pressure units in the input and output data files.
- IU1(4) defaults to a value of 1 (pressure units in atmospheres) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(5):

- IU1(5) is the specification for input and output of temperature units, where

  IU1(5) = 0 or 1 for temperature in units of degrees Celsius (°C),
  IU1(5) = 2 for temperature in units of Kelvin (K), and
  IU1(5) = 3 for temperature in units of degrees Fahrenheit (°F).

  Note: t_c °C = t_k - 273.15 K = (t_f - 32) / 1.8 °F

The unit system selected applies to all temperature units in the input and output data files.

- IU1(5) defaults to a value of 1 (temperature units in degrees Celsius) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(6):

- IU1(6) is the specification for input and output of mass units, where

IU1(6) = 0 or 1 for mass in units of grams (g),
IU1(6) = 2 for mass in units of kilograms (kg), and
IU1(6) = 3 for mass in units of pounds (lb).

Note: 1 g = 1.0×10^{-3} kg = 2.2046×10^{-3} lb

The unit system selected applies to all mass units in the input and output data files. Hence for the above selections, the corresponding mass-flow-rate units are g per time, kg per time, and lb per time, respectively.

- IU1(6) defaults to a value of 1 (mass units in grams) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(7):

- IU1(7) is the specification for input and output of permeability units, where

IU1(7) = 0 or 1 for permeability in units of square centimeters (cm^2),
IU1(7) = 2 for permeability in units of square decimeters (dm^2),
IU1(7) = 3 for permeability in units of square meters (m^2),
IU1(7) = 4 for permeability in units of square inches (in^2),
IU1(7) = 5 for permeability in units of square feet (ft^2),
IU1(7) = 6 for permeability in units of square yards (yd^2), and
IU1(7) = 7 for permeability in units of darcys (darcy).

Note: 1 cm^2 = 1.0×10^{-2} dm^2 = 1.0×10^{-4} m^2 = 1.5500×10^{-1} in^2
= 1.0764×10^{-3} ft^2 = 1.1960×10^{-4} yd^2 = 1.0×10^{8} darcy

The unit system selected applies to all permeability units in the input and output data files.

- IU1(7) defaults to a value of 1 (permeability units in square centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

NMAX:

- NMAX is the maximum number of iterations that can be performed in least squares parameter search before the program terminates. If NMAX is exceeded, an error message is displayed.
- NMAX must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (I10).
- Input example: 10000000.

RER:

- The program uses a hill-descending algorithm to obtain the least squares estimate of permeability in the domain. These computations are iterative in nature and, thus, require some closure criteria specifying the point at which an acceptable level of convergence has been achieved. RER defines a value for the relative error between consecutive permeability predictions that must be achieved before the iterative loop in the program can be exited. Ideally, output sensitivity to RER should be checked by the user.
- RER must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

B1 (Only for IOP2 = 2):

- B1 is the average thickness (in the Z-direction) of the unit between the well and the atmosphere.
- B1 must be specified only if IOP2 = 2; otherwise, leave the line blank.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.000.

XK1 (Only for IOP2 = 2):

- XK1 is an estimate for the vertical air-phase permeability in the upper unit between the well and the atmosphere. AIR2D uses XK1 as a starting value for the program search, and the computing required to obtain the solution is influenced by the initial estimate of XK1.
- XK1 must be specified only if IOP2 = 2, otherwise leave the line blank.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 numbers: (E10.3).
- Input example: 5.000E-09.

AR:

- AR is an estimate of the anisotropy ratio, k_r/k_z for isotropic domains where AR = 1.0 and for anisotropic domains where AR $\neq$ 1.0. AIR2D uses AR as a starting value for the program search, and the computing required to obtain the solution is influenced by the initial estimate of AR.
- AR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).

- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.2.

XKR:

- XKR is the estimate for horizontal permeability (k_r) of the air phase. AIR2D uses XKR as a starting value for the program search, and the computing required to obtain the solution is influenced by the initial estimate of XKR.
- XKR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 numbers: (E10.3).
- Input example: 5.000E-08.

DECR:

- This program uses a hill-descending algorithm to obtain the least squares estimate of the permeabilities of the domain. These computations are iterative in nature and, thus, require incremental adjustments to the parameter estimates in order to ensure convergence. DECR defines the decrement by which parameter estimates are decreased with each iteration. Note that DECR significantly affects the simulation time. Ideally, the user starts with a coarse value of DECR (for example DECR = 0.9) and generates permeability values. The calculated permeabilities then can be used to replace the initial estimates (XKR) and a second more refined search can be performed (for example DECR = 0.999).
- DECR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.4).
- Input example: 0.99.

DINC:

- As stated above, the program uses a hill-descending algorithm to obtain the least squares estimate of the permeabilities of the domain. These computations require incremental adjustments to the parameter estimates, and DINC defines the increment by which parameter estimates are increased. See comments on DECR for the effect of DINC on computing times.
- DINC must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.4).
- Input example: 1.01.

ZD:

- ZD is the depth from the surface to the top of the well screen when IOP2 = 1 or the depth from the bottom of upper unit to the top of well screen when IOP2 = 2. In the air-flow models, this dimension also is referred to as Hantush distance d (see figures 2 and 3).
- ZD must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 27.000.

ZL:

- ZL is the depth from the surface to the bottom of well screen when IOP2 = 1 or the depth from the bottom of upper unit to the bottom of the well screen when IOP2 = 2. In the air-flow models, this dimension also is referred to as Hantush distance l (see figures 2 and 3).
- ZL must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 58.000.

ZB:

- ZB is the depth from the surface when IOP2 = 1 or from the bottom of upper unit to the water table when IOP2 = 2. In the air-flow models, this dimension also is referred to as Hantush distance b (see figures 2 and 3).
- ZB must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 118.000.

RW:

- RW is the effective well radius. In the case of full-scale permeability tests, the effective well radius can be estimated by using the radius of the borehole.
- RW must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 3.800.

NPTS:

- NPTS is the number of probes in the domain used to monitor pressure response at a particular flow rate. NPTS is equivalent to the number of pressure measurements used to calibrate the model. Ideally, for a single simulation, NPTS should not exceed 100.
- NPTS must be specified in order to implement the air-flow model. NPTS must be input NR times along with TAIR, TSOIL, ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed two characters: (I2).
- Input example: 3.

TAIR:

- TAIR is the temperature at the surface during the full-scale permeability test.
- TAIR must be specified in order to implement the air-flow model. TAIR must be input NR times along with NPTS, TSOIL, ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 22.000.

TSOIL:

- TSOIL is the temperature at the mid-depth of the well screen during the full-scale permeability test.
- TSOIL must be specified in order to implement the air-flow model. TSOIL must be input NR times along with NPTS, TAIR, ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 17.000.

ATM:

- ATM is the prevailing atmospheric pressure during the full-scale permeability test.
- ATM must be specified in order to implement the air-flow model. ATM must be input NR times along with NPTS, TAIR, TSOIL, P3, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.992.

P3:

- P3 is the pressure measured in the well. AIR2D uses P3 to convert volumetric flow (Q4) through the well into a mass flow rate. Note that if Q4 is input as a mass flow rate, no correction is necessary, and hence, no value for P3 should be input.
- P3 must be specified only if Q4 is input as a volumetric flow rate. If Q4 is input as a mass flow rate, no value should be specified for P3. When necessary, P3 is input NR times along with NPTS, TAIR, TSOIL, ATM, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.874.

Q4:

- Q4 is the measured air-flow rate through the well. Two input options are available for Q4--mass flow rate and volumetric flow rate. When Q4 is input as a mass flow rate, no entry is be made for P3. When Q4 is input as a volumetric flow rate, P3 must be input so that AIR2D can calculate the mass flow rate from Q4. Several unit systems are available for entering mass and volumetric flow rates. AIR2D also provides the user with the option of entering mass and volumetric flow rates in terms of scale/meter readings (dimensionless). For this option, calibration data files relating the scale/meter readings to actual flow rates must be set up and specified in AFLOW (see Section 4.2.2). Any corrections to Q4 that are needed to compensate for flow measurements recorded at prevailing conditions should be performed prior to entering Q4 (corrections are instrument dependent). The program, however, does have one option for correcting rotameter measurements taken at non-standard temperature and pressure (see Section 4.2.2).
- Q4 must be specified in order to implement the air-flow model. Q4 must be input NR times along with NPTS, TAIR, TSOIL, ATM, P3, and AFLOW.
- Numeric input only is accepted (real).
- Units are dimensionless for scale reading input,
  depend on IU1(2) and IU1(3); default is cm^3/s for volumetric flow,

depend on IU1(6) and IU1(3); default is g/s for mass flow.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 39.000.

AFLOW:
- AFLOW is the name of the file containing flowmeter-calibration data.
- If, Q4 = scale/meter readings, then AFLOW must be specified; otherwise, no entry for AFLOW is required.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: CALIBGM1.CPS.

RD(I):
- RD(I) is the horizontal distance to the pressure probe in the domain from center line of the well.
- RD(I) must be specified in order to implement the air-flow model. RD(I) must be input NPTS times (once for each monitoring probe in domain) along with ZDA(I) and PHID(I) in NR data sets (one data set for each flow rate recorded).
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 3.810.

ZDA(I):
- ZDA(I) is the depth from land surface (for IOP2 = 1) or from bottom of the upper unit (for IOP2 = 2 or IOP2 = 3) to the mid-height of the monitoring probe in the domain.
- ZDA(I) must be specified in order to implement the air-flow model. ZDA(I) should be input NPTS times (once for each monitoring probe in domain) along with RD(I) and PHID(I) in NR data sets (one data set for each flow rate recorded).
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 42.500.

PHID(I):
- PHID(I) is the pressure measured at the monitoring probe. The input pressure is modified by AIR2D to account for the static-head effects resulting from the air column in the tube. AIR2D then normalizes the input pressure by dividing by the prevailing atmospheric pressure. The normalized value then is used to calibrate the air-flow models.
- PHID(I) must be specified in order to implement the air-flow model. PHID(I) should be input NPTS times (once for each probe in monitoring network) along with RD(I) and ZDA(I) in NR data sets (one data set for each flow rate recorded).
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.5).
- Input example: 0.97731.

4.2.2 Input File CALIBXX

CALIBXX specifications are as follows:

Name of file:	Specified by the user.
File contents:	Name of flowmeter, lower and upper scale limits, standard pressure and temperature for scale readings, number of correlation data points, and scale readings with corresponding flow readings.
File application:	This file is used whenever flow measurements are input in terms of scale or meter readings.
File unit number:	The program defines the CALIBxx input file as UNIT = 9.
Program input:	Data from the CALIBxx file are input in the subroutine DATAIN. The file may be read several times.
Data units:	Air-flow rates, corresponding to the scale or meter readings, must be set up by the user in the unit system adopted in the program simulation. If a unit system is not specified, air-flow input must conform to the default units (see descriptions for input variable in Section 5.2.4). Note that AIR2D accepts either volumetric or mass flow rate input, and hence, units should conform to the type of flow being input. Correlations between scale readings and flow rates in CALIBxx must be specified in ascending order (lowest flow rates first and highest flow rates last).

The structure and formatting of the CALIBxxx file is shown below.

1. Data: AF1
   Format: A12

2. Data: VAR1,VAR2
   Format: *

3. Data: PFM,TFM
   Format: *

4. Data: ICRN
   Format: *

INPUT Item 5 ICRN TIMES (once for each flowmeter data point).

5. Data: SCALE1,FLOW1
   Format: *

An example of CALIBXX is shown below:

```
                                                  Input Records
Data     Explanation                              |---+----+----+----+
Item                                              1   5    10   15   20

 1.      AF1--------------------------------------COLE-PARMER
 2.      VAR1,VAR2-------------------------------- 0.0      150.0
 3.      PFM,TFM---------------------------------- 1.000    21.11
 4.      ICRN------------------------------------- 16
```

```
5.      SCALE1,FLOW1-----(SET 1)---------------------------- 0.00     0.000
5.      SCALE1,FLOW1-----(SET 2)---------------------------- 10.00   15.983
5.      SCALE1,FLOW1-----(SET 3)---------------------------- 20.00   37.083
5.      SCALE1,FLOW1-----(SET 4)---------------------------- 30.00   57.567
5.      SCALE1,FLOW1-----(SET 5)---------------------------- 40.00   78.867
5.      SCALE1,FLOW1-----(SET 6)---------------------------- 50.00   99.617
5.      SCALE1,FLOW1-----(SET 7)---------------------------- 60.00  119.267
5.      SCALE1,FLOW1-----(SET 8)---------------------------- 70.00  138.450
5.      SCALE1,FLOW1-----(SET 9)---------------------------- 80.00  157.700
5.      SCALE1,FLOW1-----(SET 10)--------------------------- 90.00  176.783
5.      SCALE1,FLOW1-----(SET 11)---------------------------100.00  196.900
```

Note:

1. The example data set (SCALE1,FLOW1) presents information from the flowmeter Cole-Parmer calibration chart (in units of cm^3/s) for tube number: NO34-39ST.

A description of the variables required in the CALIBxx file is presented below. Flow rates, corresponding to flowmeter scale readings in the file CALIBxx, must be input in the unit system specified by the user and, ideally, should correspond to the type of flow being input (either volumetric or mass flow rates). Flowmeter scale reading and flow rates must be input in ascending order, that is, from lowest to highest values. Variables are presented in the same order as they appear in the data-input file.

AF1:

- AF1 is the name of flowmeter.
- AF1 is for descriptive purposes only and is not used in the calculations of air-flow rate. If no assignment is made to AF1, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: COLE PARMER.

VAR1:

- VAR1 is the minimum scale reading for specified flowmeter. VAR1 is used to test the input scale reading to ensure that it falls within the defined range of correlations. If the entered scale reading lies outside the recorded limits, the user is alerted to the error.
- VAR1 must be specified in order to generate air-flow rates from flowmeter-scale readings.
- Numeric input only is accepted.
- Units are dimensionless.
- Input length is unlimited (*).
- Input example: 0.0.

VAR2:

- VAR2 is the maximum scale reading for specified flowmeter. VAR2 is used to test the input scale reading to ensure that it falls within the defined range of correlations. If the entered scale reading lies outside the recorded limits, the user is alerted to the error.
- VAR2 must be specified in order to generate air-flow rates from flowmeter scale readings.
- Numeric input only is accepted.
- Units are dimensionless.
- Input length is unlimited (*).
- Input example: 150.0.

PFM:

- AIR2D provides an option to correct volumetric-flow input for nonstandard temperature and pressure conditions. The flow correction applies only to flow measurements obtained by using a rotameter (see equation 43). To perform the correction, values for PFM and TFM must be specified. To skip the correction option, leave PFM and TFM blank. PFM is the pressure at which the rotameter scale readings correspond directly to published flow rates. PFM is the standard pressure referenced on manufacture's calibration chart. Note that flow measurements obtained by using other types of flow instrumentation should be adjusted for any nonstandard effects prior to entry into AIR2D.
- PFM is required only for measurements obtained by using a rotameter; otherwise, leave it blank. If no entry is made, no correction to the volumetric flow rates will be made. If PFM and TFM are non-zero, the rotameter correction will be applied to all volumetric-flow input.
- Numeric input only is accepted.
- Units depend on IU1(4); default is atm.
- Input length is unlimited (*).
- Input example: 1.000.

TFM:

- AIR2D provides an option to correct volumetric-flow input for nonstandard temperature and pressure conditions. The flow correction applies only to flow measurements obtained by using a rotameter (see equation (34)). To perform the correction, values for PFM and TFM must be specified. To skip the correction option, leave PFM and TFM blank. TFM is the temperature at which flowmeter-scale readings correspond directly to published flow rates (for example, TFM is the standard temperature referenced on manufacture's calibration chart). Note that flow measurements obtained by using other types of flow instrumentation should be adjusted for any nonstandard effects prior to entry into AIR2D.
- TFM is required only for measurements obtained by using a rotameter; otherwise, leave it blank. If no entry is made, no correction to the volumetric-flow rates is made. If PFM and TFM are non-zero, the rotameter correction will be applied to all volumetric-flow input.
- Numeric input only is accepted.
- Units depend on IU1(5); default is °C.
- Input length is unlimited (*).
- Input example: 21.100.

ICRN:

- ICRN is the number of points representing scale-flow rate correlations (in liters per minute).
- ICRN must be specified in order to generate air-flow rates from flowmeter-scale readings.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length is unlimited (*).
- Input example: 16.

SCALE1:

- SCALE1 is the flowmeter-scale reading. Entries for SCALE1 must be input in ascending order.
- SCALE1 must be specified in order to generate air-flow rates from flowmeter-scale readings. SCALE1 is input ICRN times along with FLOW1.
- Numeric input only is accepted (real).
- Units are dimensionless.

- Input length is unlimited (*).
- Input example: 10.00.

FLOW1:

- FLOW1 is the flow rate corresponding to flowmeter-scale reading. AIR2D accepts either volumetric-flow input or mass-flow input. Entries for FLOW1 must be input in ascending order.
- FLOW1 must be specified in order to generate air-flow rates from flowmeter-scale readings. FLOW1 should be input ICRN times along with SCALE1.
- Numeric input only is accepted (real).
- Units depend on IU1(2) and IU1(3); default is cm^3/s for volumetric flow.
  depend on IU1(6) and IU1(3); default is g/s for mass flow.
- Input length is unlimited (*).
- Input example: 0.959.

4.2.3 Output File TESTFULL.OUT

TESTFULL.OUT specifications are as follows:

Name of file:	Specified by user (for example, TESTFULL.OUT).
File contents:	Project, date, well number, thickness and estimated permeabilities, well specifications, temperature, pressure, and flow measurements taken during tests, calculated mass flow, horizontal permeability, vertical permeability, leakage ratio, anisotropy ratio, error summary, and output notes.
File application:	This file is used for output from full-scale permeability analyses. Output is always displayed on the screen; hence, the name of file is required only when a permanent record of output is needed.
File unit number:	The program defines the output file as UNIT = 18.
Program output:	Output is controlled in the subroutine DATAOUT. Output from the simulation is written only when the program execution is complete.
Data units:	Data units are indicated in the tabulated output. Units conform to the user's specifications. Where no selections were made by the user, data is output in the default units.

An example of TESTFULL.OUT is provided below.

```
          PROJECT      : FULL-SCALE PERMEABILITY TEST
          SCOPE        : RESULTS OF FULL-SCALE PERMEABILITY TESTS
          TEST DATE    : 06/04/1991
          WELL NUMBER  :  9

1. MODEL INPUT SUMMARY
MODEL DOMAIN           : THICKNESS = 118.000 cm
                       : ESTIMATED HORIZONTAL PERMEABILITY =.500E-07 cm^2
                       : ESTIMATED ANISOTROPY RATIO =    1.20
UPPER Lithologic UNIT  : THICKNESS =  10.000 cm
                       : ESTIMATED PERMEABILITY =.500E-08 cm^2
WELL DEPTH (HANTUSH d) : TOP OF SCREEN =    27.00 cm
WELL DEPTH (HANTUSH l) : BOTTOM OF SCREEN =    58.00 cm
WELL RADIUS            : EFFECTIVE RADIUS =     3.80 cm
Air-flow DIRECTION     : VAPOR EXTRACTION
```

```
    2. MODEL OUTPUT SUMMARY
******************************************************************************
  AIR   SOIL    ATMOS.     SYSTEM      FLOW-    SCALE     PREVAIL.  ACTUAL
  TEMP  TEMP    PRESS.     PRESS.      METER    READING   FLOW      FLOW
  degC  degC    atm        atm         TYPE       --       cm^3/s    cm^3/s
******************************************************************************
  22.00  17.00    .992       .874       GILMONT   39.00     540.000   576.032
  22.00  17.00    .992       .916       GILMONT   29.00     403.333   420.266
  22.00  17.00    .992       .963       GILMONT   16.00     223.333   226.960
******************************************************************************

******************************************************************************
   MASS      HORIZON.   VERTICAL   LEAKAGE     ANISOTPY  MEAN OF     STD DEV
   FLOW      PERM.      PERM.     RATIO(k/b)   RATIO     ERROR IN    OF ERROR
   g/s       cm^2       cm^2        cm^2/cm      (kr/kz)   PRESS.      IN PRESS.
******************************************************************************
     .604   .774E-07   .571E-07   .154E-08     1.356    .137E-03    .243E-02
     .462   .616E-07   .399E-07   .108E-08     1.545   -.103E-03    .288E-02
     .262   .673E-07   .423E-07   .455E-08     1.593    .199E-02    .378E-02
******************************************************************************
```

4.3 AIR2D - Application to Determine Air-Phase Permeability with a Small-Scale Permeability Test

To solve an air-permeability-calibration problem by using AIR2D and a small-scale permeability test (Section 3.2), the following data files are used:

- TEST2xx - TEST2xx is used to input field data and program-control information (Section 4.3.1).
- CALIBxx - CALIBxx is used to input data points representing correlations between flowmeter-scale readings and flow rates in specified unit systems under standard conditions (Section 4.3.2).
- FRICDATA - FRICDATA is used to input data points representing Reynolds number-friction factor correlations (Section 4.3.3).

The file TEST2xx is required for small-scale permeability applications. CALIBxx is optional in most applications and is required only if flow rates are input in terms of flowmeter-scale readings. FRICDATA also is optional; its use depends on whether the friction factors are obtained from interpolation, input by the user, or calculated by using theoretical formulations. The user can specify the unit system to be used for length, volume, time, pressure, temperature, mass, and permeability. Output from the small-scale permeability simulations always is displayed on the screen. The user can also specify that the output be written to a file. This can be done either interactively or by direct entry with the data input files. Section 4.3.4 presents an example of the output obtained from the small-scale permeability simulation.

4.3.1 Input File TEST2xx

TEST2xx specifications are as follows:

Name of file:	Specified by user after invoking AIR2D (for example, TESTMINI.IN).
File contents:	Project, date, pipe identification number, direction of air flow, filenames, number of flow measurements, geologic data/model selection, units, number of iterations, closure criteria, properties of upper unit, properties of domain, model decrements/increments, Hantush values, tube diameter, tube roughness, prevailing conditions, and flow and pressure measurements.
File application:	This file inputs data used to determine small-scale permeability values. The file is required for all small-scale permeability applications.
File unit number:	The program defines the TEST2xx input file as UNIT = 8.
Program input:	Data from the TEST2xx file is input by two subroutines. General test details are accessed from the subroutine SETUP once per simulation. Flow and pressure measurements are accessed from the subroutine DATAIN several times per simulation, depending on the number of variations in flow rates (NR).
Data units:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output can be specified by the user. If no unit system is specified, units must conform to the default unit system.

The structure and formatting of file TEST2xx is as follows:

1. Data: PROJECT
   Format: A40

2. Data: DATE
   Format: A12

3. Data: WELLNUM
   Format: A12

4. Data: DINJ,AOUT,AFRIC
   Format: F10.6,2A12

5. Data: NR,IOP1,IOP2,IU1(1),IU1(2),IU1(3),IU1(4),IU1(5),IU1(6),IU1(7)
   Format: 10I5

6. Data: NMAX,RER
   Format: I10,E10.3
   IF IOP2 = 2 THEN INPUT Item 7 ELSE LEAVE BLANK LINE IF IOP2 = 1
7. Data: B1,XK1
   Format: F10.3,E10.3

8. Data: AR,XKR
   Format: F10.3,E10.3

9. Data: DECR,DINC
Format: 2F10.4

10. Data: ZD,ZL,ZB,RW,D1,AKS
Format: 5F10.3,F10.6

INPUT Items 11 and 12 NR TIMES (for example, once for each test)

11. Data: TAIR,TSOIL,ATM,P3,Q4,IQMV,AFLOW
Format: 5F10.3,I2,A12

An example of TEST2xx is shown below.

```
                                                     Input records
Data    Explanation                |---+----+----+----+----+----+----+----+----+----+----+----|
item                               1   5    10   15   20   25   30   35   40   45   50   55   60

1. PROJECT-------------------------SMALL-SCALE-PERMEABILITY TEST - RIGOROUS
2. DATE----------------------------01/21/1991
3. WELLNUM------------------------  9
4. DINJ,AOUT,AFRIC---------------- -1.0     TESTMINI.OUTFRICDATA.EXP
5. NR,IOP1,IOP2,IU1(1),..,IU1(7)-    3    1    2    1    1    1    1    1    1    1
6. NMAX,RER-----------------------   10000000 1.000E-05
7. B1,XK1-------------------------      10.000 5.000E-10
8. AR,XKR-------------------------       1.000 2.000E-08
9. DECR,DINC----------------------      0.9900    1.0100
10.ZD,ZL,ZB,RW,D1,AKS-------------      61.000    107.000    155.000      3.800      0.396 0.000
11.TAIR,TSOIL,ATM,P3,Q4,IQMV,AFLOW-     9.000     5.300     1.009     0.996    12.000  CALIBGM1.CPS
11.TAIR,TSOIL,ATM,P3,Q4,IQMV,AFLOW-     9.000     5.300     1.009     0.971    23.000  CALIBGM1.CPS
11.TAIR,TSOIL,ATM,P3,Q4,IQMV,AFLOW-     9.000     5.300     1.009     0.951    31.000  CALIBGM1.CPS
```

The variables required in the TEST2xx file are defined below. The user can select the most convenient unit systems for input and output of the data. If no unit systems are specified, input must conform to the default unit systems. Variables are presented in the order in which they appear in the data-input file.

PROJECT:

- PROJECT is the project title or description that identifies the test data.
- PROJECT is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to PROJECT, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 40 characters: (A40).
- Input example: SMALL-SCALE PERMEABILITY TEST.

DATE:

- DATE is the date of the small-scale permeability field tests.
- DATE is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to DATE, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: 01/21/1991.

WELLNUM:

- WELLNUM is the identification number assigned to the probe used in the field test.
- WELLNUM is for descriptive purposes only and is not needed to implement the air-flow models. If no assignment is made to WELLNUM, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: 9.

DINJ:

- DINJ is the variable that records whether air was withdrawn (DINJ = -1.0) or injected during the small-scale permeability test (DINJ = 1.0).
- DINJ must be specified in order to implement the air-flow model. If the absolute value of DINJ does not equal 1.0, an error message will be displayed.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: -1.0 (for air withdrawal).

AOUT:

- AOUT is the name of the file used for output data.
- AOUT is optional. If AOUT is not specified, the program will prompt the user to specify whether output should be displayed on the screen or written to a data file. If the user selects a data file for output, the program prompts the user for the name of the output file. If no name is assigned to AOUT, the output will be displayed on the screen and not saved.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: TESTMINI.OUT.

AFRIC:

- AFRIC is the name of the file that contains data points representing Reynolds number- friction factor correlations (see Section 4.3.3). If the word THEORY is input, the program uses theoretical formulations to predict the friction factor that corresponds to the prevailing Reynolds number. Note that output is sensitive to friction-factor assignments.
- AFRIC is optional. If AFRIC is not specified in the data-input file, the program will prompt the user to specify whether Reynolds number-friction factor data will be input by way of a data file, interactively, or calculated from theoretical formulations. If the user selects a data file for the input, the program prompts the user for the name of the input file. If an assignment is not made to AFRIC, the user must specify interactively the friction factor that corresponds to the displayed Reynolds number. If the user selects the theoretical method of predicting friction factor, the program automatically assigns the word THEORY to AFRIC. This may be done directly by the user as described above.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: FRICDATA

NR:

- NR is the number of variations in well injection/withdrawal air-flow rates for which pressure measurements in the domain were obtained. For a single application of AIR2D, NR cannot exceed 10.
- NR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 3.

IOP1:

- IOP1 is the variable that records whether the domain is isotropic, $k_r \approx k_z$ (IOP1 = 1), or anisotropic, $k_r \neq k_z$ (IOP1 = 2). For small-scale permeability tests, isotropic conditions must be assumed in order to apply the analytical solutions (for example, $k \approx k_r \approx k_z$). Hence, IOP1 = 1 is the only valid selection. Note that the program will overwrite selections for IOP1 ≠ 1 whenever a small-scale permeability analysis is being performed.
- Regardless of the values specified for IOP1, the program will default the setting to IOP1=1 (isotropic domain) for small-scale permeability analyses.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 0 for isotropic domain (the only valid selection).

IOP2:

- IOP2 records whether an upper unit (between the well and the atmosphere) is absent (IOP2 = 1), or present (IOP2 = 2). The selection made for IOP2 determines the analytical solution that is used by AIR2D.
- IOP2 defaults to a value of 1 (no upper unit present and domain open to atmosphere model) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1 (for no upper unit).

IU1(1):

- IU1(1) is the specification for input and output of length units, where

IU1(1) = 0 or 1 for length in units of centimeters (cm),
IU1(1) = 2 for length in units of decimeters (dm),
IU1(1) = 3 for length in units of meters (m),
IU1(1) = 4 for length in units of inches (in.),
IU1(1) = 5 for length in units of feet (ft), and
IU1(1) = 6 for length in units of yards (yd).

Note: 1 cm = 1.0×10^{-1} dm = 1.0×10^{-2} m = 3.937×10^{-1} in.
= 3.281×10^{-2} ft = 1.0937×10^{-2} yd.

The unit system selected applies to all length units in the input and output data files.

- IU1(1) defaults to a value of 1 (length units in centimeters) when no value is specified.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(2):

- IU1(2) is the specification for input and output of volume units, where

IU1(2) = 0 or 1 for volume in units of cubic centimeters (cm^3),
IU1(2) = 2 for volume in units of liters (L),
IU1(2) = 3 for volume in units of cubic meters (m^3),
IU1(2) = 4 for volume in units of cubic inches (in^3),
IU1(2) = 5 for volume in units of cubic feet (ft^3),
IU1(2) = 6 for volume in units of cubic yards (yd^3), and
IU1(2) = 7 for volume in units of gallons (gal).

Note: $1\ cm^3 = 1.0 \times 10^{-3} L = 1.0 \times 10^{-6} m^3 = 6.1023 \times 10^{-2} in^3$
$= 3.5314 \times 10^{-5} ft^3 = 1.3079 \times 10^{-6} yd^3 = 2.6417 \times 10^{-4} gal$

The unit system selected applies to all volume units in the input and output data files. Note that the volumetric unit system does not have to correspond to the length unit system.

- IU1(2) defaults to a value of 1 (volume units in cubic centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(3):

- IU1(3) is the specification for input and output of time units, where

IU1(3) = 0 or 1 for time in units of seconds (s),
IU1(3) = 2 for time in units of minutes (min),
IU1(3) = 3 for time in units of hours (hr),
IU1(3) = 4 for time in units of days (d), and
IU1(3) = 5 for time in units of years (yr).

Note: $1\ s = 1.6667 \times 10^{-2} min = 2.7778 \times 10^{-4} hr$
$= 1.1574 \times 10^{-5} d = 3.1688 \times 10^{-8} yr$

The unit system selected applies to all time units in the input and output data files. Hence, for the above selections, the corresponding volumetric or mass-flow-rate output units are flow per second, flow per minute, flow per hour, flow per day, or flow per year, respectively.

- IU1(3) defaults to a value of 1 (time units in seconds) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(4):

- IU1(4) is the specification for input and output of pressure units, where

  IU1(4) = 0 or 1 for pressure in units of atmospheres (atm),
  IU1(4) = 2 for pressure in units of millimeters of mercury (mm-Hg),
  IU1(4) = 3 for pressure in units of inches of water (in-H_2O),
  IU1(4) = 4 for pressure in units of kilopascals (kPa), and
  IU1(4) = 5 for pressure in units of pound per square inch (lb/in^2).

  Note: 1 atm = 760 mm-Hg = 406.38 in-H_2O = 101.325 kPa = 14.70 lb/in^2

  The unit system selected applies to all pressure units in the input and output data files.
- IU1(4) defaults to a value of 1 (pressure units in atmospheres) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(5):

- IU1(5) is the specification for input and output of temperature units, where

  IU1(5) = 0 or 1 for temperature in units of degrees Celsius (°C),
  IU1(5) = 2 for temperature in units of Kelvin (K), and
  IU1(5) = 3 for temperature in units of degrees Fahrenheit (°F).

  Note: t_c °C = t_k - 273.15 K = (t_f - 32) / 1.8 °F

  The unit system selected applies to all temperature units in the input and output data files.
- IU1(5) defaults to a value of 1 (temperature units in degrees Celsius) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(6):

- IU1(6) is the specification for input and output of mass units, where

  IU1(6) = 0 or 1 for mass in units of grams (g),
  IU1(6) = 2 for mass in units of kilograms (kg), and
  IU1(6) = 3 for mass in units of pounds (lb).

  Note: 1 g = 1.0 x 10^{-3} kg = 2.2046 x 10^{-3} lb

  The unit system selected applies to all mass units in the input and output data files. Hence for the above selections, the corresponding mass-flow-rates units are g per time, kg per time, and lb per time, respectively.

- IU1(6) defaults to a value of 1 (mass units in grams) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(7):

- IU1(7) is the specification for input and output of permeability units, where

  IU1(7) = 0 or 1 for permeability in units of square centimeters (cm^2),
  IU1(7) = 2 for permeability in units of square decimeters (dm^2),
  IU1(7) = 3 for permeability in units of square meters (m^2),
  IU1(7) = 4 for permeability in units of square inches (in^2),
  IU1(7) = 5 for permeability in units of square feet (ft^2),
  IU1(7) = 6 for permeability in units of square yards (yd^2), and
  IU1(7) = 7 for permeability in units of darcys (darcy).

  Note: $1\ cm^2 = 1.0 \times 10^{-2}\ dm^2 = 1.0 \times 10^{-4}\ m^2 = 1.5500 \times 10^{-1}\ in^2$
  $= 1.0764 \times 10^{-3}\ ft^2 = 1.1960 \times 10^{-4}\ yd^2 = 1.0 \times 10^{8}$ darcy

  The unit system selected applies to all permeability units in the input and output data files.
- IU1(7) defaults to a value of 1 (permeability units in square centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

NMAX:

- NMAX is the maximum number of iterations that can be performed before the least-squares-parameter-fitting algorithm is terminated. If NMAX is exceeded, an error message is displayed.
- NMAX must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (I10).
- Input example: 10000000.

RER:

- The program uses a hill-descending algorithm to obtain the least-squares estimate of the permeability in the domain. These computations are iterative in nature and, thus, require some closure criteria that specifies the point at which an acceptable level of convergence has been achieved. RER defines a value for the relative error between consecutive model predictions that must be achieved before the iterative loop in the program can be exited.
- RER must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

B1:

- B1 is the average thickness (in the Z-direction) of the upper unit (unit between the well and the atmosphere).
- B1 must be specified only if IOP2 = 2 or IOP2 = 3; otherwise, leave it blank.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.000.

XK1:

- XK1 is the air permeability of the air phase in the upper unit (unit between the well and the atmosphere, if applicable). Unlike the full-scale analysis, no fit is generated by AIR2D for XK1 during the small-scale permeability simulations because only one data point is available. Consequently, the air-permeability estimate for the domain depends on the fixed value selected for XK1.
- XK1 must be specified if IOP2 = 2; otherwise, leave it blank.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 numbers: (E10.3).
- Input example: 5.000E-10.

AR:

- AR is an estimate of the anisotropy ratio (defined as the horizontal permeability of the air phase divided by the vertical permeability of the air phase or k_r/k_z) in the domain under investigation. In small-scale permeability tests, the assumption is made that $k \approx k_r \approx k_z$ in the geologic strata in which the vapor probe is positioned; hence, AR = 1.0 is the only valid selection. Note that the program will overwrite the user selection and assign AR = 1.0 if a small-scale permeability analysis is performed.
- Regardless of the values specified for AR, the program will default the setting to AR = 1.0 (isotropic domain) for small-scale permeability analyses.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.0 (the only valid selection).

XKR:

- XKR is an estimate of composite air permeability ($k = k_r = k_z$) in the domain. AIR2D uses XKR as a starting value for the air permeability. Although the output from AIR2D is independent of XKR, the convergence time taken to reach the final permeability value can be affected by the initial estimate. For small-scale permeability analyses, vertical permeability (k_z) in the domain is assumed to equal k_r. The AIR2D estimate for k = XKR depends on the estimate for k' = XK1 (see comments for XK1 above).
- XKR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 numbers: (E10.3).
- Input example: 2.000E-08.

DECR:

- The program uses a hill-descending algorithm to obtain the least-squares estimate of the air permeability in the domain. These computations require incremental adjustments to the permeability estimates. DECR defines the decrement by which parameter estimates are decreased with each iteration. Note that DECR significantly affects the simulation time. Ideally, the user should start with a coarse value of DECR (for example, DECR = 0.99) and generate air-permeability values. The generated values then can be used to replace the initial estimates (XKR) and a second, more refined search can be performed (for example, DECR = 0.999).
- DECR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.4).
- Input example: 0.9900.

DINC:

- The computations in a program that uses a hill-descending algorithm require incremental adjustments to the air-permeability estimates. DINC defines the increment by which parameter estimates are increased. See previous comments on DECR.
- DINC must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.4).
- Input example: 1.0100.

ZD:

- ZD is the depth from the land surface to the top of the probe screen (when IOP2 = 1) or the depth from the bottom of the upper unit to the top of the probe screen (when IOP2 = 2 or IOP2 = 3). In the air-flow models, this dimension also is referred to as Hantush distance d (see figures 2 and 3).
- ZD must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 61.000.

ZL:

- ZL is the depth from the land surface to the bottom of the probe screen (when IOP2 = 1) or the depth from the bottom of upper unit to the bottom of the probe screen (when IOP2 = 2 or IOP2 = 3). In the air-flow models, this dimension also is referred to as Hantush distance l (see figures 2 and 3).
- ZL must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 107.000.

ZB:

- ZB is the depth from the land surface (when IOP2 = 1) or from the bottom of the upper unit (when IOP2 = 2 or IOP2 = 3) to the water table. In the air-flow models, this dimension also is referred to as Hantush distance b (see figures 2 and 3).
- ZB must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 155.000.

RW:

- RW is the effective well radius. For small-scale permeability tests, the radius of the pack surrounding the probe, which is approximately equal to the radius of the borehole, is used.
- RW must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 3.800.

D1:

- D1 is the internal diameter of the tubing that connects the vapor probe to the land surface.
- D1 must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.396.

AKS:

- AKS is the relative roughness of the tubing that connects the vapor probe to the surface. AKS is needed to calculate the friction factor in the transitional and turbulent flow regimes (flows with Reynolds numbers > 2000) by using the Colebrook-White relation (see equation 39). The value AKS varies with the type of material used to construct the tube.
- AKS is only specified if (1) the Reynolds numbers that describe the flow in the pipe are greater than 2000 and (2) the friction factor is evaluated by using theoretical formulations. A value of AKS = 0, which implies a smooth surface, can be used if no other information is available.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: 0.05 for rough surfaces, or, 0.00 for smooth surfaces.

TAIR:

- TAIR is the temperature at the land surface during the small-scale permeability test.
- TAIR must be specified in order to implement the air-flow model. TAIR must be input NR times along with TSOIL, ATM, P3, Q4, IQMV, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 9.000.

TSOIL:

- TSOIL is the temperature at middepth of the vapor probe during the test.
- TSOIL must be specified in order to implement the air-flow model. TSOIL must be input NR times along with TAIR, ATM, P3, Q4, IQMV, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 5.300.

ATM:

- ATM is the prevailing atmospheric pressure during the small-scale permeability test.
- ATM must be specified in order to implement the air-flow model. ATM must be input NR times along with TAIR, TSOIL, P3, Q4, IQMV, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.009.

P3:

- P3 is the system pressure measured at the surface. P3 is used to evaluate the pressure at the probe during small-scale permeability tests. The probe pressure then is used to calibrate the air-flow models. For IQMV = 0, P3 along with Q4 is used to determine mass flow rate out of the well. P3 should be measured at several different flow rates at steady-state conditions. Note that a special feature of AIR2D is that when P3 < 0.25 atm, P3 represents the pressure differential between the small-scale permeability system pressure and the prevailing atmospheric pressure. This allows pressure to be input directly as manometer-deflection measurements.
- P3 must be specified in order to implement the air-flow model. P3 must be input NR times along with TAIR, TSOIL, ATM, Q4, IQMV, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.013.

Q4:

- Q4 is the measured air-flow rate through the well. Two input options are available for Q4--mass-flow rate and volumetric flow rate. When Q4 is input as a mass flow rate, the variable IQMV must be set to 1. When Q4 is input as a volumetric flow rate, the variable IQMV must be set to 0 or left blank. AIR2D will calculate the mass flow rate from Q4 and P3. Several unit systems are available for entering mass and volumetric flow rates. AIR2D also provides the user with the option of entering mass and volumetric flow rates in terms of scale/meter readings (dimensionless). For this option, calibration data files relating the scale/meter readings to actual flow rates must be created and specified in AFLOW (see Section 4.3.2). Any changes to Q4 to correct flow measurements at prevailing conditions for non-standard temperatures and pressures should be made prior to entering Q4 (corrections will be instrument dependent). The program, however, does have one option for correcting rotameter measurements made at nonstandard temperatures and pressures.
- Q4 must be specified in order to implement the air-flow model. Q4 must be input NR times along with TAIR, TSOIL, ATM, P3, IQMV, and AFLOW.

- Numeric input only is accepted (real).
- Units, dimensionless for scale reading,
  - depend on IU1(2) and IU1(3); default is cm^3/s for volumetric flow.
  - depend on IU1(6) and IU1(3); default is g/s for mass flow.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 12.000.

IQMV:

- IQMV records whether flow input represents volumetric flow rates (IQMV = 0) or mass flow rates (IQMV = 1). For IQMV = 0, AIR2D calculates the mass flow through the well by using Q4 and P3.
- IQMV defaults to a value of 0 (Q4 is treated as volumetric-flow input) if no value is specified by the user. When necessary, IQMV is input NR times along with TAIR, TSOIL, ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed two characters: (I2).
- Input example: 0

AFLOW:

- AFLOW is the name of the file containing the flowmeter-calibration data.
- If Q4 represents the flowmeter scale readings, AFLOW must be specified; otherwise, no entry is required for AFLOW.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: CALIBGM1.CPS.

4.3.2 Input File CALIBxx

For small-scale permeability simulations, if flow data is entered as flowmeter-scale readings, a calibration (CALIBxx) file is required to relate flowmeter-scale readings to actual flow rates in the specified unit system. If flow data is entered as actual flow rates, a calibration file is not required. Section 4.2.2 gives detailed information on the set up of the CALIBxx files.

4.3.3 Input File FRICxx

FRICxx specifications are as follows:

Name of file:	Specified by user (for example, FRICDATA).
File contents:	Number of data points representing Reynolds number-friction factor correlation.
File application:	This file provides Reynolds number-friction factor correlations using data obtained experimentally or from theoretical formulations.
File unit number:	The program defines the FRICxx input file as UNIT = 10.
Program input:	Data from the FRICxx file is input in the subroutine SETUP and FRIKF. The file is read for each separate flow rate.
Data units:	The Reynolds number and the friction factor are dimensionless.

The structure of the FRICxx file is given below.

1. Data: NV
   Format: I3

INPUT Item 2, NV TIMES (once for each calibration data set)

2. Data: RENO(I),FXN(I)
   Format: *

An example FRICDATA file is given below.

Data item	Explanation	Input records 1 5 10 15 20
1.	AF1	5
2.	RENO(I),FXN(I)	1015.59 0.063018
2.	RENO(I),FXN(I)	2539.69 0.030641
2.	RENO(I),FXN(I)	4436.31 0.028712
2.	RENO(I),FXN(I)	7529.48 0.026737
2.	RENO(I),FXN(I)	10495.98 0.024638

The friction-factor file FRICxx contains data points that define the correlation between Reynolds numbers and friction factors for air flow through the tubing used in the small-scale permeability tests. Alternatively, AIR2D can determine the friction factor theoretically as explained in Section 3.3.2. AIR2D also can be used to analyze experiments conducted on tubing (Section 4.4) and construct the data for file FRICxx. AIR2D fits a cubic spline through the data points contained in the FRICxx file to interpolate friction factors over a range of flow conditions. Reynolds numbers corresponding to friction factors in the file FRICxx must be input for a range of values that encompasses flow rates encountered during the small-scale permeability tests. Data points must be input in ascending order (lowest Reynolds number first).

Variable definitions are as follows:

NV:

- NV is the number of data points in the file.
- NV must be specified. If a value less than one is assigned to NV, the program will disregard the interpolating option in the program and prompt the user for the friction factor that corresponds to the Reynolds number.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 3 characters: (I3).
- Input example: 6.

RENO(I):

- RENO() is the Reynolds number that corresponds to the friction factor.
- RENO() is input NV times along with FXN().
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length is unlimited (*).
- Input example: 1015.59.

FXN(I):

- FXN() is the friction factor that corresponds to specified Reynolds numbers. AIR2D uses the friction factor to determine pressure at the vapor probe from the surface measurements by correcting for losses due to friction.
- FXN() is input NV times along with RENO().
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length is unlimited (*).
- Input example: 0.063018.

4.3.4 Output File TESTMINI.OUT

TESTMINI.OUT specifications are as follows:

Name of file:	Specified by user (for example, TESTMINI.OUT).
File contents:	Project, date, well number, thickness, and estimated permeability of model domain and lithologic units, probe specifications, air extraction or injection, prevailing temperature and pressure, flow and pressure measurements taken during tests, calculated Reynolds number, friction factor, probe pressure, and air-phase permeability.
File application:	This file is used for output from small-scale permeability analyses. Output is always displayed on the screen; hence, name of file is only required when a permanent record of output is needed.
File unit number:	The program defines the output file as UNIT = 18.
Program output:	Output is controlled by subroutine DATAOUT. Output from the simulation is written only when the program is complete.
Data units:	Data units are indicated in the tabulated output. Units conform to the user specifications. Where no selections were made by the user, data is output in the default units.

An example of TESTMINI.OUT is as follows:

```
          PROJECT     : SNALL-SCALE-PERMEABILITY TEST
          SCOPE       : RESULTS OF SMALL-SCALE-PERMEABILITY TESTS
          TEST DATE   : 01/21/1991
          WELL NUMBER :  9

 1. MODEL INPUT SUMMARY
 MODEL DOMAIN           : THICKNESS = 155.000 cm
                        : ESTIMATED HORIZONTAL PERMEABILITY =.200E-07 cm^2
                        : ESTIMATED ANISOTROPY RATIO =   1.00
 UPPER   UNIT  : THICKNESS =  10.000 cm
                        : ESTIMATED PERMEABILITY =.500E-09 cm^2
 PROBE DEPTH (HANTUSH d): TOP OF PROBE =   61.00 cm
 PROBE DEPTH (HANTUSH l): BOTTOM OF PROBE =  107.00 cm
 WELL RADIUS            : EFFECTIVE RADIUS =    3.80 cm
 PIPE DIAMETER          : DIAMETER =  .396 cm
 AIR FLOW DIRECTION     : VAPOR EXTRACTION
```

```
    2. MODEL OUTPUT SUMMARY
******************************************************************************
  AIR    SOIL     ATMOS.      SYSTEM       FLOW      SCALE      PREVAIL.   ACTUAL
  TEMP   TEMP     PRESS.      PRESS.       METER     READING    FLOW       FLOW
  degC   degC     atm         atm          TYPE        --       cm^3/s     cm^3/s
******************************************************************************
   9.00   5.30    1.009        .996        GILMONT    12.00     170.000    166.251
   9.00   5.30    1.009        .971        GILMONT    23.00     320.000    316.947
   9.00   5.30    1.009        .951        GILMONT    31.00     430.000    430.352
******************************************************************************
******************************************************************
  MASS       REYNOLD    FRIC.      PROBE        AIR          SUM OF
  FLOW         NO.      FACTOR     PRESS.    PERMEABILITY     ERROR
  g/s          --        --        atm          cm^2         SQUARED
******************************************************************
    .2073    3873.6     .0270     1.0024     .4094E-07     .2256E-08
    .3854    7199.4     .0273      .9939     .3322E-07     .3744E-08
    .5125    9574.0     .0249      .9887     .3289E-07     .1685E-09
******************************************************************
```

4.4 AIR2D - Application to Determine Friction Factor

AIR2D can create data to be stored in the file FRICxx (Section 4.3.3). The file used as input will depend upon whether the evaluation is experimental or theoretical.

- TEST3axx - is used to input experimental data and program control information (Section 4.4.1).
- TEST3bxx - is used to input theoretical data and program control information (Section 4.4.2).
- CALIBxx - is used to input correlation data between flowmeter-scale readings and flow rates, in liters per minute, under standard conditions (Section 4.4.3).

One of the files, TEST3axx or TEST3bxx, is always required for friction-factor evaluations. In the case of the experimental evaluation of the friction factor, TEST3axx contains information collected at the time and location of the test. In the case of the theoretical prediction of the friction factor, TEST3bxx contains ranges of Reynolds numbers for which friction factors are to be evaluated. Note that this option may be invoked directly during small-scale permeability analyses by specifying THEORY for variable AFRIC (Section 4.3.1).

The data file CALIBxx only applies to the experimental determination of the friction factor. CALIBxx is required only when flow rates are input as flowmeter-scale readings. Output from the small-scale permeability simulations is always displayed on the screen. The user can specify that the output be written to a file. This can be done either interactively or by direct entry with the data files. Section 4.4.4 presents examples of the output obtained from both experimental and theoretical evaluations. Section 4.4.5 presents a summarized output data file (FRICDATA) that can be used in small-scale permeability simulations. Note that friction-factor determinations are not required for full-scale permeability analyses since pressures in the monitoring probes are measured under static conditions.

4.4.1 Experimental Friction Factor Input File TEST3axx

File specifications are given below.

Name of file: Specified by the user.

File contents: Project, date, pipe number, flow direction, filenames, number of flow measurements, units, number of iterations, closure criteria, equipment dimensions, prevailing conditions, and flow and pressure measurements.

File application: This file is used to input the data required to evaluate the friction factor by using experimental techniques.

File unit number: The program defines the TEST3axx input file as UNIT = 8.

Program input: Data from the TEST3axx file is input in two subroutines. General details of the test are accessed from the subroutine SETUP once per simulation. Flow and pressure measurements or specifications are accessed from the subroutine DATAIN several times per simulation, depending on the number of variations in flow rates (NR).

Data units: Unit systems for length, volume, time, pressure, temperature, and mass can be specified; otherwise, units must conform to the default unit system.

The structure of the TEST3axx file is shown below.

1. Data: PROJECT
   Format: A40

2. Data: DATE
   Format: A12

3. Data: PIPENO
   Format: A12

4. Data: DINJ,AOUT,AFRIC
   Format: F10.6,2A12

5. Data: NR,IU1(1),IU1(2),IU1(3),IU1(4),IU1(5),IU1(6)
   Format: 7I5

6. Data: NMAX,RER
   Format: I10,E10.3

7. Data: D1,XMAX
   Format: 2F10.3

INPUT Item 8, NR TIMES (once for each test)

8. Data: TAIR,ATM,P3,Q4,IQMV,AFLOW
   Format: 4F10.3,I2,A12

An example of the input file is given below:

```
                                                      Input records
Data    Explanation                          |----+----+----+----+----+----+----+----+----+----+
item                                         1    5    10   15   20   25   30   35   40   45   50

 1. PROJECT--------------------------------FRICTION FACTOR EVALUATION FROM TESTS
 2. DATE-----------------------------------08/25/1989
 3. PIPENO--------------------------------- # 1
 4. DINJ,AOUT,AFRIC------------------------ -1.0      FRIC1.OUT   FRICDATA.EXP
 5. NR,IU1(1),IU1(2),...,IU1(6)------------  5    1    1    1    3    1    1
 6. NMAX,RER-------------------------------  10000000 1.000E-05
 7. D1,XMAX--------------------------------    0.396    91.440
 8. TAIR,ATM,P3,Q4,IQMV,AFLOW--(1)---        19.000   407.450     0.563     2.200  CALIBGM1.CP1
 8. TAIR,ATM,P3,Q4,IQMV,AFLOW--(2)---        19.000   407.450     1.500     8.000  CALIBGM1.CP1
 8. TAIR,ATM,P3,Q4,IQMV,AFLOW--(3)---        19.000   407.450     4.313    14.500  CALIBGM1.CP1
 8. TAIR,ATM,P3,Q4,IQMV,AFLOW--(4)---        19.000   407.450    11.750    25.000  CALIBGM1.CP1
 8. TAIR,ATM,P3,Q4,IQMV,AFLOW--(5)---        19.000   407.450    21.500    35.500  CALIBGM1.CP1
```

Definitions of the variables required in the TEST3axx file are presented below. The user can select the most convenient unit systems for input and output of data. If no unit systems are specified, input must conform to the default unit systems.

PROJECT:

- PROJECT is the project title or description identifying the test data.
- PROJECT is for descriptive purposes only and is not needed to implement the pipe-flow model. If no assignment is made to PROJECT, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 40 characters: (A40).
- Input example: FRICTION FACTOR EVALUATION FROM TESTS.

DATE:

- DATE is the date of the friction-factor field tests for experimental analysis or the date of simulation for theoretical analysis.
- DATE is for descriptive purposes only and is not needed to implement the pipe-flow model. If no assignment is made to DATE, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: 8/25/1989.

PIPENO:

- PIPENO is the identification number assigned to the pipe being investigated.
- PIPENO is for descriptive purposes only and is not needed to implement the pipe-flow model. If no assignment is made to PIPENO, a blank line must be left in the data file.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: # 1.

DINJ:

- DINJ is the variable that records whether air was withdrawn (DINJ = -1.0) or air was injected (DINJ = 1.0) during the experiment.
- DINJ must be specified in order to implement the pipe-flow model. If the absolute value of DINJ does not equal 1.0, an error message will be displayed.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: -1.0 (for air withdrawal).

AOUT:

- AOUT is the name of the file to be used for output data.
- AOUT is optional. If AOUT is not specified, the program will prompt the user to specify whether output should be displayed on the screen or written to a data file. If the user selects a data file for output, the program prompts the user for the name of the output file. If a name is not assigned to AOUT, the output will be displayed on the screen and not saved.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: FRIC1.OUT.

AFRIC:

- AFRIC is the name of the file to which Reynolds numbers corresponding to friction factor data are written. The output directed to this file differs from that in AOUT above. AFRIC is formatted so that it can be used for FRICDATA input in small-scale permeability simulations (see Section 4.4.4).
- AFRIC is optional. If AFRIC is not specified, the program will prompt the user interactively to specify whether or not the Reynolds number-friction factor correlations should be output to a data file. If the user selects the data file output option, the program prompts the user for the name of the output file and sends the appropriate information to that address. If no name is assigned to AFRIC, data in the form of the FRICDATA input file will not be formatted.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: FRICDATA.

NR:

- During the experimental tests, pressure declines over a length of pipe are measured at various flow rates. NR is the number of variations in flow rate for which pressure measurements were obtained.
- NR must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 5.

IU1(1):

- IU1(1) is the specification for input and output of length units, where

IU1(1) = 0 or 1 for length in units of centimeters (cm),
IU1(1) = 2 for length in units of decimeters (dm),
IU1(1) = 3 for length in units of meters (m),
IU1(1) = 4 for length in units of inches (in),
IU1(1) = 5 for length in units of feet (ft), and
IU1(1) = 6 for length in units of yards (yd).

Note: 1 cm = 1.0×10^{-1} dm = 1.0×10^{-2} m = 3.937×10^{-1} in.
= 3.281×10^{-2} ft = 1.0937×10^{-2} yd.

The unit system selected applies to all length units in the input and output data files.

- IU1(1) defaults to a value of 1 (length units in centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(2):

- IU1(2) is the specification for input and output of volume units, where

IU1(2) = 0 or 1 for volume in units of cubic centimeters (cm^3),
IU1(2) = 2 for volume in units of liters (L),
IU1(2) = 3 for volume in units of cubic meters (m^3),
IU1(2) = 4 for volume in units of cubic inches (in^3),
IU1(2) = 5 for volume in units of cubic feet (ft^3),
IU1(2) = 6 for volume in units of cubic yards (yd^3), and
IU1(2) = 7 for volume in units of gallons (gal).

Note: 1 cm^3 = 1.0×10^{-3} L = 1.0×10^{-6} m^3 = 6.1023×10^{-2} in^3
= 3.5314×10^{-5} ft^3 = 1.3079×10^{-6} yd^3 = 2.6417×10^{-4} gal

The unit system selected applies to all volume units in the input and output data files. Note that the volumetric unit system does not have to correspond to the length unit system.

- IU1(2) defaults to a value of 1 (volume units in cubic centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(3):

- IU1(3) is the specification for input and output of time units, where

  IU1(3) = 0 or 1 for time in units of seconds (s),
  IU1(3) = 2 for time in units of minutes (min),
  IU1(3) = 3 for time in units of hours (hr),
  IU1(3) = 4 for time in units of days (d), and
  IU1(3) = 5 for time in units of years (yr).

  Note: 1 s = 1.6667×10^{-2} min = 2.7778×10^{-4} hr
  = 1.1574×10^{-5} d = 3.1688×10^{-8} yr

  The unit system selected applies to all time units in the input and output data files. Hence, for the above selections, the corresponding volumetric or mass-flow-rate output units are flow per second, flow per minute, flow per hour, flow per day, or flow per year, respectively.
- IU1(3) defaults to a value of 1 (time units in seconds) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(4):

- IU1(4) is the specification for input and output of pressure units, where

  IU1(4) = 0 or 1 for pressure in units of atmospheres (atm),
  IU1(4) = 2 for pressure in units of millimeters of mercury (mm-Hg),
  IU1(4) = 3 for pressure in units of inches of water (in-H_2O),
  IU1(4) = 4 for pressure in units of kilopascals (kPa), and
  IU1(4) = 5 for pressure in units of pound per square inch (lb/in^2).

  Note: 1 atm = 760 mm-Hg = 406.38 in-H_2O = 101.325 kPa = 14.70 lb/in^2

  The unit system selected applies to all pressure units in the input and output data files.
- IU1(4) defaults to a value of 1 (pressure units in atmospheres) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(5):

- IU1(5) is the specification for input and output of temperature units, where

  IU1(5) = 0 or 1 for temperature in units of degrees Celsius (°C),
  IU1(5) = 2 for temperature in units of Kelvin (K), and
  IU1(5) = 3 for temperature in units of degrees Fahrenheit (°F).

  Note: t_c °C = t_k - 273.15 K = (t_f - 32) / 1.8 °F

The unit system selected applies to all temperature units in the input and output data files.

- IU1(5) defaults to a value of 1 (temperature units in degrees Celsius) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(6):

- IU1(6) is the specification for input and output of mass units, where

  IU1(6) = 0 or 1 for mass in units of grams (g),
  IU1(6) = 2 for mass in units of kilograms (kg), and
  IU1(6) = 3 for mass in units of pounds (lb).

  Note: 1 g = 1.0×10^{-3} kg = 2.2046×10^{-3} lb

  The unit system selected applies to all mass units in the input and output data files. Hence for the above selections, the corresponding mass-flow-rate units are g per time, kg per time, and lb per time, respectively.
- IU1(6) defaults to a value of 1 (mass units in grams) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

NMAX:

- NMAX is the maximum number of iterations that can be performed before the program is terminated. If NMAX is exceeded, an error message is displayed.
- NMAX must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (I10).
- Input example: 10000000.

RER:

- The program performs a number of iterative calculations that require some closure criteria specifying the point at which an acceptable level of convergence has been achieved. RER defines a value for the relative error between consecutive model predictions that must be achieved before the iterative loop in the program can be exited.
- RER must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

D1:

- D1 is the internal diameter of tubing being investigated.
- D1 must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.396.

XMAX:

- XMAX is the length of tubing being investigated.
- XMAX must be specified in order to implement the pipe flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 91.440.

TAIR:

- TAIR is the temperature of the air during the friction-factor tests.
- TAIR must be specified in order to implement the pipe-flow model. TAIR is input NR times along with ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 19.0.

ATM:

- ATM is the prevailing atmospheric pressure during friction-factor tests.
- ATM must be specified in order to implement the pipe-flow model. ATM is input NR times along with TAIR, P3, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.003.

P3:

- P3 is the system pressure measured at the tube end near the pneumatic pump. P3 is used to determine the pressure drop along the pipe resulting from friction loss. For IQMV = 0, P3 along with Q4 is used to determine mass flow rate through the pipe. Ideally, P3 should be measured at several different flow rates at steady-state conditions. Note that a special feature of AIR2D is that for P3 < 0.25 atmospheres, P3 represents the pressure differential between the system pressure and the prevailing atmospheric pressure (that is, pressure loss over length of pipe). This allows for pressure input directly in terms of manometer deflection measurements.
- P3 must be specified in order to implement the pipe-flow model. P3 is input NR times along with TAIR, TSOIL, ATM, Q4, and AFLOW.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.001.

Q4:

- Q4 is the measured air-flow rate through the tube. Two input options are available for Q4. When Q4 is input as a mass flow rate, the variable IQMV must be set to 1. When Q4 is input as a volumetric-flow rate, the variable IQMV must be set to 0 (or left blank). AIR2D will calculate the mass flow rate from Q4 and P3. A number of unit systems are available for entering mass and volumetric flow rates.
  AIR2D also provides the user with the option of entering mass and volumetric flow rates in terms of scale/meter readings. For this option, calibration data files relating the scale/meter readings to actual flow rates, must be formatted and specified in AFLOW (see Section 4.4.3). Any corrections to Q4 to compensate for flow measurements recorded at prevailing conditions are performed prior to entering Q4 (corrections will be instrument dependent). The program, however, does have one option for correcting rotameter measurements taken at nonstandard temperature and pressure.
- Q4 must be specified in order to implement the air-flow model. Q4 must be input NR times along with TAIR, ATM, P3, IQMV, and AFLOW.
- Numeric input only is accepted (real).
- Units are dimensionless - for scale reading input.
  Limits depend on IU1(2) and IU1(3); default is cm^3/s - for volumetric flow.
  Limits depend on IU1(6) and IU1(3); default is g/s - for mass flow.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 2.200.

IQMV:

- IQMV records whether flow input represents volumetric flow rates (IQMV=0) or mass flow rates (IQMV = 1). For IQMV = 0, AIR2D calculates the mass flow through the well by using Q4 and P3.
- IQMV defaults to a value of 0 (that is, Q4 is treated as volumetric flow input) if no value is specified by the user. When necessary, IQMV is input NR times along with TAIR, ATM, P3, Q4, and AFLOW.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed two characters: (I2).
- Input example: 0.

AFLOW:

- AFLOW is the name of the file containing the flowmeter calibration data.
- If Q4 = flowmeter-scale readings, AFLOW must be specified, otherwise, no entry for AFLOW is required.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: CALIBGM1.CPS.

4.4.2 Theoretical Friction Factor Input File TEST3bxx

File specifications are as follows:

Name of file:	Specified by user
File contents:	Relative roughness, output filename, number of Reynolds numbers specified, number of iterations permitted, closure criteria, diameter of pipe, Reynolds numbers.
File application:	This file is used to input data required to evaluate the friction factor by using theoretical techniques. The file is required only when user specifies DIRECT MODE for input of data.
File unit number:	The program defines the TEST3bxx input file as UNIT = 8.
Program input:	Data from the TEST3bxx file is entered in two subroutines. General test details are accessed from the subroutine SETUP once per simulation. Reynolds numbers are accessed from the subroutine DATAIN several times per simulation, depending on the number specified (NR).
Data units:	A unit system for length input and output can be specified by the user. If length units are not specified, lengths must be input in centimeters. All remaining entries in TEST3bxx are dimensionless.

The structure of the TEST3bxx file is shown below.

1. Data: AKS,AFRIC
   Format: F10.6,A12

2. Data: NR,IU1(1)
   Format: 2I5

3. Data: NMAX,RER
   Format: I10,E10.3

4. Data: D1
   Format: F10.3

INPUT Item 5, NR TIMES (once for each Reynolds number)

5. Data: RE
   Format: F10.3

An example file is given below.

```
                                                 Input records
Data Explanation                             |---+----+----+----+----+----+
item                                         1   5   10   15   20   25   30
 1.     AKS,AFRIC----------------------------  0.000   FRICDATA.THY
 2.     NR,IU1(1) ---------------------------    6    1
 3.     NMAX,RER-----------------------------  10000000 1.000E-05
 4.     D1-----------------------------------     0.396
 5.     RE---------(VALUE 1) ----------------  1000.000
 5.     RE---------(VALUE 2) ----------------  2000.000
 5.     RE---------(VALUE 3) ----------------  4000.000
```

```
5.      RE————————(VALUE 4)————————————————    5000.000
5.      RE————————(VALUE 5)————————————————    7500.000
5.      RE————————(VALUE 6)————————————————   10500.000
```

Definitions of the variables required in the TEST3bxx file are presented below. The user can select the most convenient unit systems for input and output of data. If no unit systems are specified, input must conform to the default unit systems.

AKS:

- AKS is the relative roughness of the pipe. AKS is needed to calculate friction factor in the transitional and turbulent flow regimes (that is, flows with Reynolds numbers > 2000) by using the Colebrook-White relation (see equation 39). AKS varies with the type of material from which the tube is constructed.
- AKS must be specified if the Reynolds numbers that describe flow in the pipe are greater than 2000. A value of AKS = 0, implying a smooth surface, can be used if no other information is available.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: 0.050 rough surfaces.
  0.000 smooth surfaces.

AFRIC:

- AFRIC is the name of the file to which Reynolds number in relation to friction factor data are written. The output directed to this file is formatted to the requirements of the FRICDATA input file used in small-scale permeability simulations (see Section 4.3.3).
- AFRIC is optional. If AFRIC is not specified, the program will prompt the user interactively to specify whether or not friction factor-Reynolds number correlations should be output to a data file. If the user selects the data-file output option, the program prompts the user for the name of the output file and sends the appropriate information to that address. If no name is assigned to AFRIC, the output will be displayed on the screen and no permanent records will be generated.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: FRICDATA.

NR:

- NR is the number of specified Reynolds numbers for which friction factors are to be generated.
- NR must be specified in order to implement the theoretical models.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 6.

IU1(1):

- IU1(1) is the specification for input and output of length units, where

  IU1(1) = 0 or 1 for length in units of centimeters (cm),
  IU1(1) = 2 for length in units of decimeters (dm),
  IU1(1) = 3 for length in units of meters (m),
  IU1(1) = 4 for length in units of inches (in.),
  IU1(1) = 5 for length in units of feet (ft), and
  IU1(1) = 6 for length in units of yards (yd).

  Note: 1 cm = 1.0×10^{-1} dm = 1.0×10^{-2} m = 3.937×10^{-1} in.
  = 3.281×10^{-2} ft = 1.0937×10^{-2} yd.

  The unit system selected applies to all length units in the input and output data files.
- IU1(1) defaults to a value of 1 (length units in centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

NMAX:

- NMAX is the maximum number of iterations that can be performed before the program is terminated. If NMAX is exceeded, an error message is displayed.
- NMAX must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (I10).
- Input example: 10000000.

RER:

- The program performs a number of iterative calculations that require some closure criteria specifying the point at which an acceptable level of convergence has been achieved. RER defines a value for the relative error between consecutive model predictions that must be achieved before the iterative loop in the program can be exited. In addition, RER is used in the Colebrook-White equation to adjust friction-factor estimates during each iteration.
- RER must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

D1:

- D1 is the inside diameter of the tubing being investigated.
- D1 must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 0.396.

RE:

- RE is the Reynolds number specified by the user for which friction factors are determined by using theoretical formulations.
- RE must be specified in order to implement the pipe-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1000.000.

4.4.3 Input File CALIBxx

Experimental evaluation of the friction factor is based upon flow measurements. The flow measurements can be entered either as flow rates or as flowmeter scale readings. For flow input as flow rates, no calibration (CALIBxx) files are required. For flow input as flowmeter scale readings, the relation between the scale readings and actual flow rates in the specified unit system is entered in the CALIBxx file. Section 4.2.2 gives detailed information on the formatting of the CALIBxx files. Note that the experimental friction-factor data file (Section 4.4.1) uses CALIBGM1.CP1 rather than CALIBGM1.CPS that appears in the small-scale permeability simulation (Section 4.2.1). The various files are used to account for the different pressure-unit systems used in the two simulations.

4.4.4 Output File FRIC1.OUT

Two options are available for the output of the results of the friction-factor analysis. The first option (FRIC1.OUT), discussed below, lists simulation results in a format similar to the small-scale permeability output. The second option discussed in Section 4.4.5 lists an abbreviated form of the output in a format compatible with small-scale permeability test input requirements. FRIC1.OUT output files are available only for friction factor analyses that uses experimental procedures. The option is invoked by specifying a filename for the variable AOUT in the friction-factor input file (see Section 4.4.1) or through interactive selections. FRICDATA output files can be generated for either experimental or theoretical simulations. This option is invoked by specifying a filename for the variable AFRIC in the friction-factor input file (see Section 4.4.1) or through interactive selections.

During FRICDATA generation, output is written directly to the file specified by the user. For simulations based on experimental data, FRICDATA output is not displayed on the screen. For simulations based on theoretical predictions, however, FRICDATA output is displayed on the screen as the computations proceed.

File specifications are given below.

Name of file:	Specified by the user (for example, FRIC1.OUT)
File contents:	Project, date, pipe identification number, pipe length, pipe diameter, direction of air flow, prevailing temperature and pressure, measured pressure and flow in system, calculated mass flow rate, Reynolds number, friction factor, and friction factor for laminar case.
File application:	This file is used for output from experimental friction-factor analyses. Output is always displayed on the screen; hence, the name of the file is only required when a permanent record of output is needed.

File unit number: The program defines the output file as UNIT = 18.

Program output: Output is controlled in the subroutine DATAOUT. Output from the simulation is written only when program execution is complete.

Data units: Data units are indicated in the tabulated output. Units conform to those used in the input data. If no units were specified, output units correspond to the default unit settings.

An example file is given below.

```
                  PROJECT        : FRICTION FACTOR EVALUATION FROM TESTS

                  SCOPE          : FRICTION FACTOR USING EXPERIMENTAL METHODS
                  TEST DATE      : 08/25/1989
                  PIPE ID NUMBER: # 1
                  PIPE LENGTH    : 91.440 cm
                  PIPE DIAMETER  : .396 cm
        AIR FLOW DIRECTION       : VAPOR EXTRACTION

        1. MODEL OUTPUT SUMMARY
*****************************************************************************
  AIR   SOIL    ATMOS.      SYSTEM      FLOW     SCALE    PREVAIL. 0 ACTUAL
  TEMP  TEMP    PRESS.      PRESS.      METER    READING  FLOW       FLOW
  degC  degC    "H2O        "H2O        TYPE       --     cm^3/s     cm^3/s
*****************************************************************************
  19.00  19.00 407.450   406.887       GILMONT    2.20     46.334     46.138
  19.00  19.00 407.450   405.950       GILMONT    8.00    116.000    115.645
  19.00  19.00 407.450   403.137       GILMONT   14.50    203.334    203.416
  19.00  19.00 407.450   395.700       GILMONT   25.00    348.333    351.735
  19.00  19.00 407.450   385.950       GILMONT   35.50    491.667    502.700
*****************************************************************************


*************************************
 MASS     REYNOLD   FRIC.     FRIC.
 FLOW      NO.      FACTOR    FACTOR
 g/s       --       (Calc)    (Laminar)
*************************************
  .0555    1015.6    .0630     .0630
  .1388    2539.7    .0306     .0252
  .2424    4436.3    .0287     .0144
  .4115    7529.5    .0267     .0085
  .5736   10496.0    .0246     .0061
*************************************
```

4.4.5 Output File FRICDATA

FRICDATA output can be generated from experimental or theoretical determinations of the friction factor. The information written to the FRICDATA file is a summary of the information presented in Section 4.4.4. The file contains friction factor-Reynolds number data from the simulations. If generated, the FRICDATA file can be used for direct input of friction-factor information during the small-scale permeability simulations (see Section 4.3.3).

File Specifications are as follows:

Name of file: Specified by the user (for example, FRICDATA).

File contents: Number of friction factor-Reynolds number correlations, Reynolds number with corresponding friction factors determined from experimental or theoretical methods.

File application: This file is used for output from experimental or theoretical friction-factor analyses. Output is displayed on the screen for theoretical analyses but not for experimental analyses. Filenames can be specified when permanent records of output are needed.

File unit number: The program defines the output file as UNIT = 11.

Program output: Output is controlled in the subroutine PIPEF for experimental analyses. For theoretical analyses, output is controlled in the subroutine FRIKF. Output from the simulation is written with each application of the subroutine.

Data units: Output values are all dimensionless (Reynolds numbers and friction factors).

An example output file is given below.

```
5
 1015.59   .063017
 2539.70   .030640
 4436.32   .028711
 7529.48   .026737
10496.00   .024638
```

4.4.6 Comparison of Experimental and Theoretical Friction-Factor Determinations

Friction-factor evaluation for air flow in pipes can be performed by using either experimental or theoretical methods. The program AIR2D can be used to implement either approach. A number of assumptions and simplifications are implicit in each technique, however. Figure 6 shows graphically the experimental predictions based on data collected at the research site in Galloway Township, New Jersey, and the theoretical predictions based on the Hagen-Poiseuille (37) and Colebrook-White (39) equations. Experimental predictions are presented for five different lengths of pipe--91.0 cm, 189.0 cm, 305 cm, 405 cm, and 680 cm.

Figure 6 indicates that friction factors decrease with increasing pipe lengths. This trend results from the decreasing influence of minor pressure losses as discussed in Section 3.3.2.d. Figure 6 also indicates that the correlation between experimental and theoretical predictions of friction factor for the pipe configuration used at the Galloway research site is poor. The poor correlation indicates that for narrow tubing minor losses could be accounted for in the theoretical evaluations of the friction factor. The small-scale permeability model has been found to be sensitive to friction-factor estimates. The user ideally should always test the effect of friction-factor selection on model output.

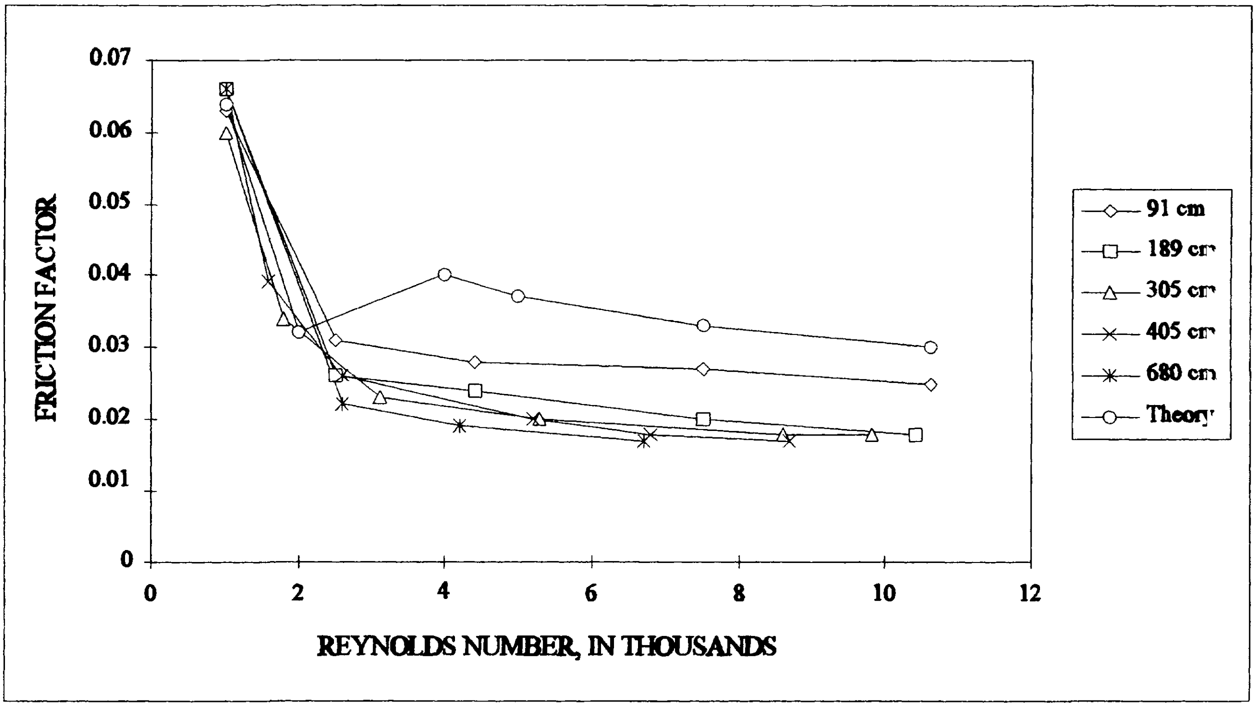


Figure 6. Friction-factor predictions using experimental and theoretical procedures.

4.5 AIR2D - Application to Predict Pressure and Flow Assuming Air-Phase Permeability

AIR2D can be applied to implement the air-flow models in a prediction mode, as described in Section 2. Pressure and air flow at specified locations in the unsaturated zone are calculated with estimated air-permeability values for the horizontal (k_r) and vertical (k_z) directions and, if applicable, for an overlying unit (k'). For this application, the following data file is required.

- TEST4xx - is used to input simulation data and program-control information (Section 4.5.1).

Note that when using AIR2D in the prediction mode, pressure and volumetric flow rate at the well cannot be independently specified because the well boundary condition is given as a constant mass flow rate which, for air behaving as an ideal gas, is proportional to their product. For a given mass flow rate, AIR2D will compute air pressure at the well, which will imply a total volumetric flow in the well. Several iterations may be required to obtain pressure and flow predictions in the model domain for a specific well pressure or well volumetric flow rate. The procedure involves modifying input values for QM for each simulation, until the pressure and (or) flow at the well match the desired values.

Output is not displayed on the screen because of the potentially large volumes of data. Instead, the information is written directly to output files. Unless the user specifies otherwise, simulation predictions are output as follows:

- pressure predictions in the domain are written to the file PVSR.OUT (see Section 4.5.2),

- volumetric flow predictions in the domain are written to the file VVSR.OUT (see Section 4.5.3),
- mass flow predictions in the domain are written to the file MVSR.OUT (see Section 4.5.4), and
- pressure and flow values at the well are written to the file WELL.OUT (see Section 4.5.5).

Three options are available for generating pressure and flow output in the model domain. Pressure, volumetric flow, and mass flow may be output:

(1) along a horizontal line (along A-B in Figure 7);
(2) along a vertical line (along B-C in Figure 7);
(3) in a cross section (bounded by A-B-C-D in Figure 7).

For each of the above options, radial and (or) vertical distances are required to define the range of output. Starting points, end points, and length intervals in the horizontal and vertical directions that must be specified by the user are illustrated in figure 7.

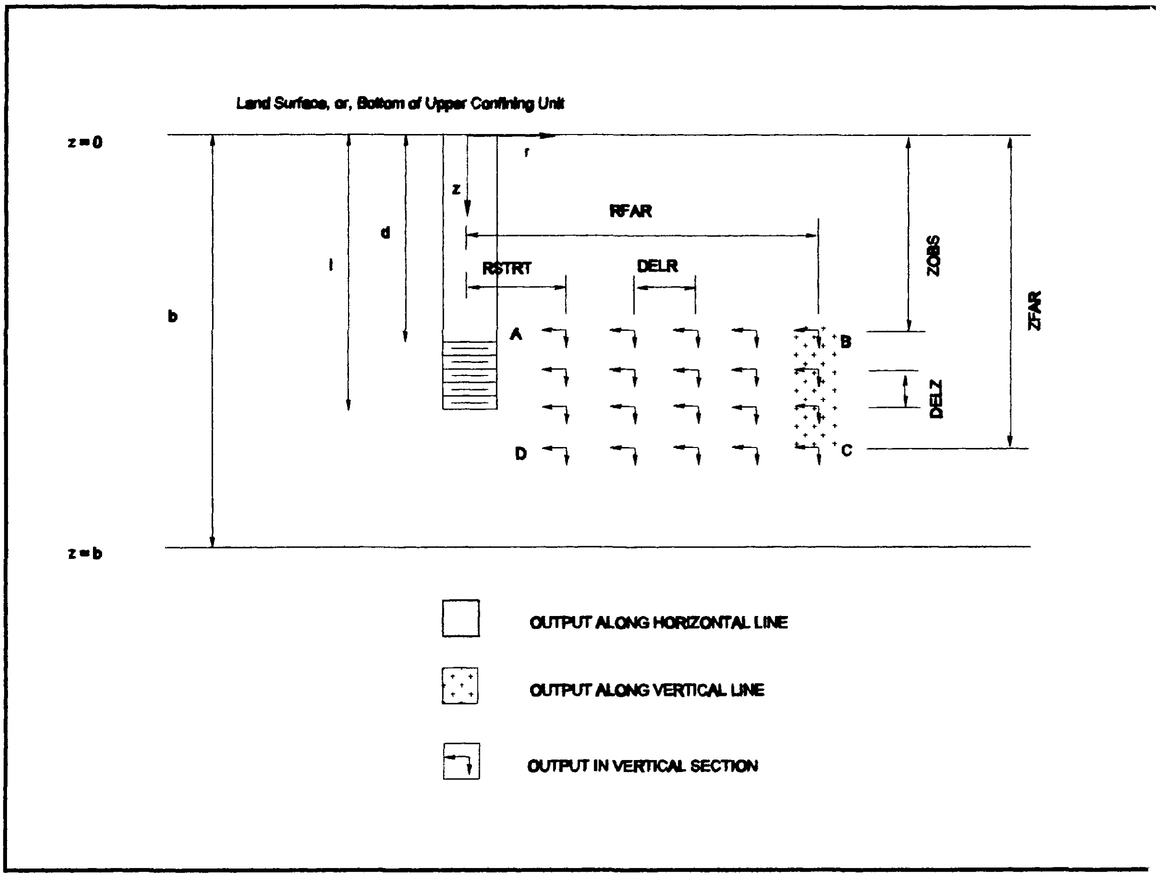


Figure 7. Output options for pressure and flow predictions.

4.5.1 Input File TEST4xx

Specifications for TEST4xx are shown below.

Name of file:	Specified by the user.
File contents:	Air injection or withdrawal, number of flow rates specified, geologic data/model selection, unit system, number of iterations, closure criteria, upper unit thickness and vertical permeability, domain anisotropy ratio and horizontal permeability, Hantush values, temperature, atmospheric pressure, mass air-flow rate, air-phase porosity, output option, names of output files, geometric range of output in horizontal and vertical directions.
File application:	This file contains input data used to predict pressure and flow distributions in the domain from analytical solutions to the air-flow equation. The file is always required for prediction mode simulations.
File unit number:	The program defines the TEST4xx input file as UNIT = 8.
Program input:	Data from the TEST4xx file is entered in two subroutines. General test details are accessed from the subroutine SETUP once per simulation. Flow and pressure measurements are accessed from the subroutine DATAIN several times per simulation, depending on the number of variations in flow rates (NR).
Data unit:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output may be specified by the user. If no unit system is specified, units must conform to the default unit systems for each input value.

The structure of the TEST4xx file is

1. Data: DINJ
   Format: F10.6

2. Data: NR,IOP1,IOP2,IU1(1),IU1(2),IU1(3),IU1(4),IU1(5),IU1(6),IU1(7)
   Format: 10I5

3. Data: NMAX,RER,RERF
   Format: I10,2E10.3

IF IOP2 = 2 or IOP2 = 3 (upper unit is present) THEN
INPUT Item 4 ELSE LEAVE BLANK LINE IF IOP2 = 1

4. Data: B1,XK1
   Format: F10.3,E10.3

5. Data: AR,XKR
   Format: F10.3,E10.3

6. Data: ZD,ZL,ZB,RW
   Format: 4F10.3

INPUT Items 7, 8, and 9 NR TIMES (once for each flow rate QM)

7. Data: TSOIL,ATM,QM
   Format: 3F10.3

8. Data: IOPS,OPVSR,OVVSR,OMVSR,OWELL
   Format: I5,4A12

IF IOPS = 1 (horizontal line output) THEN INPUT Item 9a

9a. Data: ZOBS,RSTRT,DELR,RFAR
    Format: 4F10.3

ELSE, IF IOPS = 2 (vertical line output) THEN INPUT Item 9b

9b. Data: ZOBS,RFAR,DELZ,ZFAR
    Format: 4F10.3

ELSE, IF IOPS = 3 (vertical slice output) THEN INPUT ITEM 9c

9c . Data: ZOBS,RSTRT,DELR,RFAR,DELZ,ZFAR
    Format:6F10.3

An example input file is given below.

```
                                                 Input records
Data    Explanation                      |---+----+----+----+----+----+----+----+----+----+-----
item                                     1   5    10   15   20   25   30   35   40   45
 1.     DINJ-------------------------     -1.0
 2.     NR,IOP1,IOP2,IU1(1),.,IU1(7)-    3    2    2    1    1    1    1    1    1    1
 3.     NMAX,RER,RERF----------------   10000000 1.000E-05 1.000E-05
 4.     B1,XK1-----------------------      20.000 1.000E-10
 5.     AR,XKR-----------------------       2.000 1.000E-08
 6.     ZD,ZL,ZB,RW------------------     100.000   160.000   260.000    10.000
 7.     TSOIL,ATM,QM------(OPTION 1)-      10.000     1.000     1.000
 8.     IOPS,OPVSR,OVVSR,OMVSR,OWELL-      1P11.OUT     V11.OUT     M11.OUT     W11.OUT
 9a.    ZOBS,RSTRT,DELR,RFAR---------     130.000    20.000    10.000   250.000
 7.     TAIR,ATM,QM-------(OPTION 2)-      10.000     1.000     1.000
 8.     IOPS,OPVSR,OVVSR,OMVSR,OWELL-      2P12.OUT     V12.OUT     M12.OUT     W12.OUT
 9b.    ZOBS,RFAR,DELZ,ZFAR----------     100.000   100.000    10.000   160.000
 7.     TAIR,ATM,QM-------(OPTION 3)-      10.000     1.000     1.000
 8.     IOPS,OPVSR,OVVSR,OMVSR,OWELL-      3P13.OUT     V13.OUT     M13.OUT     W13.OUT
 9c.    ZOBS,RSTRT,DELR,RFAR,DELZ,ZFAR    100.000    20.000    10.000   250.000    10.000     160.000
```

Definitions of the variables required in the TEST4xx file are presented below. The user can select the most convenient unit systems for input and output of data. If no unit systems are specified, input must conform to the default unit systems.

DINJ:

- DINJ is the variable that records whether air is withdrawn (DINJ = -1.0) or air is injected (DINJ = 1.0) during air-flow simulation.
- DINJ must be specified in order to implement the air-flow model. If absolute value of DINJ does not equal 1.0, an error message will be displayed.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.6).
- Input example: 1.0 (for air injection).

NR:

- NR is the number of variations in mass flow rate, QM, specified by the user for which the pressure and flow in the domain are to be calculated.
- NR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 3.

IOP1:

- IOP1 is the variable that records whether the domain is isotropic, $k_r \approx k_z$, (IOP1 = 1) or anisotropic, $k_r \neq k_z$, (IOP1 = 2).
- If IOP1 is not specified, the program will default to the setting IOP1 = 1, (an isotropic domain).
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 2 (for anisotropic domain).

IOP2:

- IOP2 records whether an upper unit between the well and the atmosphere is absent (IOP2=1) or present (IOP2 = 2). The selection of IOP2 also determines the analytical solution that is used by AIR2D.
- IOP2 defaults to a value of 1 (no upper unit present and domain open to atmosphere model) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1 for no upper unit.

IU1(1):

- IU1(1) is the specification for input and output of length units, where

  IU1(1) = 0 or 1 for length in units of centimeters (cm),
  IU1(1) = 2 for length in units of decimeters (dm),
  IU1(1) = 3 for length in units of meters (m),
  IU1(1) = 4 for length in units of inches (in.),
  IU1(1) = 5 for length in units of feet (ft), and
  IU1(1) = 6 for length in units of yards (yd).

  Note: 1 cm = 1.0×10^{-1} dm = 1.0×10^{-2} m = 3.937×10^{-1} in
  = 3.281×10^{-2} ft = 1.0937×10^{-2} yd.

  The unit system selected applies to all length units in the input and output data files.
- IU1(1) defaults to a value of 1 (length units in centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(2):

- IU1(2) is the specification for input and output of volume units, where

  IU1(2) = 0 or 1 for volume in units of cubic centimeters (cm^3),
  IU1(2) = 2 for volume in units of liters (L),
  IU1(2) = 3 for volume in units of cubic meters (m^3),
  IU1(2) = 4 for volume in units of cubic inches (in^3),
  IU1(2) = 5 for volume in units of cubic feet (ft^3),
  IU1(2) = 6 for volume in units of cubic yards (yd^3), and
  IU1(2) = 7 for volume in units of gallons (gal).

  Note: $1\ cm^3 = 1.0 \times 10^{-3} L = 1.0 \times 10^{-6} m^3 = 6.1023 \times 10^{-2} in^3$
  $= 3.5314 \times 10^{-5} ft^3 = 1.3079 \times 10^{-6} yd^3 = 2.6417 \times 10^{-4} gal$

  The unit system selected applies to all volume units in the input and output data files. Note that the volumetric unit system does not have to correspond to the length unit system.
- IU1(2) defaults to a value of 1 (volume units in cubic centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(3):

- IU1(3) is the specification for input and output of time units, where

  IU1(3) = 0 or 1 for time in units of seconds (s),
  IU1(3) = 2 for time in units of minutes (min),
  IU1(3) = 3 for time in units of hours (hr),
  IU1(3) = 4 for time in units of days (d), and
  IU1(3) = 5 for time in units of years (yr).

  Note: $1\ s = 1.6667 \times 10^{-2} min = 2.7778 \times 10^{-4} hr$
  $= 1.1574 \times 10^{-5} d = 3.1688 \times 10^{-8} yr$

  The unit system selected applies to all time units in the input and output data files. Hence, for the above selections, the corresponding volumetric or mass-flow-rate output units are flow per second, flow per minute, flow per hour, flow per day, or flow per year respectively.
- IU1(3) defaults to a value of 1 (time units in seconds) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(4):

- IU1(4) is the specification for input and output of pressure units, where

  IU1(4) = 0 or 1 for pressure in units of atmospheres (atm),
  IU1(4) = 2 for pressure in units of millimeters of mercury (mm-Hg),

IU1(4) = 3 for pressure in units of inches of water (in-H_2O),
IU1(4) = 4 for pressure in units of kilopascals (kPa), and
IU1(4) = 5 for pressure in units of pound per square inch (lb/in^2).

Note: 1 atm = 760 mm-Hg = 406.38 in-H_2O = 101.325 kPa = 14.70 lb/in^2

The unit system selected applies to all pressure units in the input and output data files.

- IU1(4) defaults to a value of 1 (pressure units in atmospheres) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(5):

- IU1(5) is the specification for input and output of temperature units, where

IU1(5) = 0 or 1 for temperature in units of degrees Celsius (°C),
IU1(5) = 2 for temperature in units of Kelvin (K), and
IU1(5) = 3 for temperature in units of degrees Fahrenheit (°F).

Note: t_c °C = t_k - 273.15 K = (t_f - 32) / 1.8 °F

The unit system selected applies to all temperature units in the input and output data files.

- IU1(5) defaults to a value of 1 (temperature units in degrees Celsius) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(6):

- IU1(6) is the specification for input and output of mass units, where

IU1(6) = 0 or 1 for mass in units of grams (g),
IU1(6) = 2 for mass in units of kilograms (kg), and
IU1(6) = 3 for mass in units of pounds (lb).

Note: 1 g = 1.0 x 10^{-3} kg = 2.2046 x 10^{-3} lb

The unit system selected applies to all mass units in the input and output data files. Hence for the above selections, the corresponding mass-flow-rates units are g per time, kg per time, and lb per time, respectively.

- IU1(6) defaults to a value of 1 (mass units in grams) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

IU1(7):

- IU1(7) is the specification for input and output permeability units, where

  IU1(7) = 0 or 1 for permeability in units of square centimeters (cm^2),
  IU1(7) = 2 for permeability in units of square decimeters (dm^2),
  IU1(7) = 3 for permeability in units of square meters (m^2),
  IU1(7) = 4 for permeability in units of square inches (in^2),
  IU1(7) = 5 for permeability in units of square feet (ft^2),
  IU1(7) = 6 for permeability in units of square yards (yd^2), and
  IU1(7) = 7 for permeability in units of darcys (drcy).

  Note: 1 cm^2 = 1.0×10^{-2} dm^2 = 1.0×10^{-4} m^2 = 1.5500×10^{-1} in^2
  = 1.0764×10^{-3} ft^2 = 1.1960×10^{-4} yd^2 = 1.0×10^{8} drcy

  The unit system selected applies to all permeability units in the input and output data files.
- IU1(7) defaults to a value of 1 (permeability units in square centimeters) when no value is specified by the user.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

NMAX:

- NMAX is the maximum number of terms summed to obtain convergence of the series solution. If NMAX is exceeded, an error message is displayed.
- NMAX must be specified in order to implement the air-flow model.
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (I10).
- Input example: 10000000.

RER:

- RER is the closure criteria that specifies acceptable convergence of the series solution for pressure.
- RER must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

RERF:

- RERF is the closure criteria that specifies acceptable convergence of the series solution for flow.
- RERF must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-05.

B1 (ONLY FOR IOP2 = 2):

- B1 is the average thickness of the upper unit (unit between the well and the atmosphere).
- B1 must only be specified if IOP2 = 2 (upper unit is present); otherwise, leave line blank.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 20.000.

XK1 (ONLY FOR IOP2 = 2):

- XK1 is the vertical permeability of the air phase in the upper unit (between the well and the atmosphere).
- XK1 must be specified only if IOP2 = 2; otherwise, leave line blank.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 characters: (E10.3).
- Input example: 1.000E-10.

AR:

- AR is the anisotropy ratio (horizontal permeability of the air phase divided by vertical permeability of the air phase, or k_r/k_z) in the domain under investigation. In isotropic domains, AR = 1.0, whereas in anisotropic domains, AR ≠ 1.0.
- AR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units are dimensionless.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 2.000.

XKR:

- XKR is the horizontal permeability (k_r) of the air phase in the modeled domain. AIR2D generates vertical permeability values (k_z) for the domain directly from the quotient k_r/AR.
- XKR must be specified in order to implement the air-flow model.
- Numeric input only is accepted (exponential).
- Units depend on IU1(7); default is cm^2.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.000E-08.

ZD:

- ZD is the depth from the land surface to the top of well screen (when IOP2 = 1) or the depth from the bottom of upper unit to the top of well screen (when IOP2 = 2 or IOP2 = 3). In the air-flow models, this dimension also is referred to as Hantush distance d (refer to figures 2 and 3).
- ZD must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 100.000.

ZL:

- ZL is the depth from the land surface to the bottom of the well screen (when IOP2 = 1) or depth from the bottom of upper unit to the bottom of the well screen (when IOP2 = 2 or IOP2 = 3). In the air-flow models, this dimension also is referred to as Hantush distance l (refer to figures 2 and 3).
- ZL must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 160.00.

ZB:

- ZB is the depth from the land surface to the water table (when IOP2 = 1) or from the bottom of upper unit to the water table (when IOP2 = 2 or IOP2 = 3). In the air-flow models, this dimension also is referred to as Hantush distance b (refer to figures 2 and 3).
- ZB must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 260.00.

RW:

- RW is the effective well radius. If a well pack is used, RW equals the radius of the borehole.
- RW must be specified in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.000.

TSOIL:

- TSOIL is the average air temperature prevailing during operation of the vapor-extraction system. TSOIL is required to adjust air properties, such as viscosity, which are temperature dependent.
- TSOIL must be specified in order to implement the air-flow model. TSOIL must be input NR times along with ATM and QM.
- Numeric input only is accepted (real).
- Units depend on IU1(5); default is °C.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.000.

ATM:

- ATM is the atmospheric pressure. ATM is used to convert normalized pressure output from the air-flow model to absolute values and to define the land-surface-boundary condition.
- ATM must be specified in order to implement the air-flow model. ATM must be input NR times along with TAIR and QM.
- Numeric input only is accepted (real).
- Units depend on IU1(4); default is atm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.000.

QM:

- QM is the mass flow rate of air through the well. For a specified QM, the model generates pressure and volumetric flow at the well, corresponding to geologic conditions.
- QM must be specified in order to implement the air-flow model. QM should be input NR times.
- Numeric input only is accepted (real).
- Units depend on IU1(6) and IU1(2); default is g/s.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 1.000.

IOPS:

- IOPS determines the nature of the pressure and flow output. For IOPS = 1, output is generated along a horizontal line in the model domain. For IOPS = 2, output is generated along a vertical line in the model domain. For IOPS = 3, output is generated within a vertical section of the model domain. The selection of IOPS determines the geometric input needed to define the range of pressure and flow output (see figure 7).
- IOPS must be specified in order to implement the air-flow model. IOPS should be input NR times (once for each mass flow rate).
- Numeric input only is accepted (integer).
- Units are dimensionless.
- Input length cannot exceed five characters: (I5).
- Input example: 1.

OPVSR:

- OPVSR is the name of the output file containing pressure predictions for the domain at specified depths and radial distances from the center line of the well for each of the NR simulations. Output is generated according to the user's selection of IOPS.
- OPVSR input is optional. If no entry is made, pressure output will be written to the file PVSR.OUT. This default setting also is activated during interactive simulations. Note that with multiple simulations (NR > 1), information from earlier simulations may be overwritten unless different output names for OPVSR are specified by the user.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: P1130.OUT.

OVVSR:

- OVVSR is the name of the file containing the horizontal and vertical components of volumetric flow (specific discharge) in the model domain at specified depths and radial distances from the center line of the well for each of the NR simulations.
- OVVSR input is optional. If no entry is made, volumetric-air-flow output will be written to the file VVSR.OUT. This default setting also is activated during interactive simulations Note that with multiple simulations (NR>1), information from earlier simulations is overwritten unless different output names for OVVSR are specified by the user.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: V1130.OUT.

OMVSR:

- OMVSR is the name of the file containing the horizontal and vertical components of mass-flow-rate output (mass specific discharge) at specified depths and radial distances from the center line of the well. Output is organized according to the user selection of IOPS.
- OMVSR input is optional. If no entry is made, mass-flow output will be written to the file MVSR.OUT. This default setting also is activated during interactive simulations. Note that with multiple simulations (NR>1), information from earlier simulations is overwritten unless different output names for OMVSR are used.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: M1130.OUT.

OWELL:

- OWELL is the name of the file containing pressure and flow output at the well. Output values are calculated at the mid-depth of the well screen. Output represents the pressure and volumetric flow rate that correspond to the mass flow rate at the well specified by the user.
- OWELL input is optional. If no entry is made, pressure and flow output at the well will be written to the file WELL.OUT. This default setting also is activated during interactive simulations. Note that with multiple simulations (NR>1), information from earlier simulations is overwritten unless different output names for OWELL are used.
- Alpha or numeric input is accepted.
- Units are dimensionless.
- Input length cannot exceed 12 characters: (A12).
- Input example: W1130.OUT.

ZOBS:

- ZOBS is the depth from the land surface to the top of the zone of interest (when IOP2 = 1) or the depth from the bottom of the upper unit to the top of the zone of interest (see figure 7). For IOPS = 1, ZOBS represents the depth to the horizontal line along which pressure and flow values are output. For IOPS = 2, ZOBS represents the depth to the top of the vertical line along which pressure and flow values are output. For IOPS = 3, ZOBS represents the depth to the top of the vertical section along which pressure and flow values are output.
- ZOBS must be specified to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 130.000.

RSTRT:

- RSTRT is a spatial limit in the radial direction that defines the distance to the point nearest the well for which pressure and flow output are generated (see figure 7). The distance is relative to the center line of the well, and the minimum value permitted must exceed the effective well radius (RW). For IOPS = 1 and IOPS = 3, RSTRT represents the horizontal distance from the well centerline to the start of the pressure and flow output line and the domain, respectively. For IOPS = 2, RSTRT is not used because the horizontal distance to the output line is defined by RFAR (for IOPS = 2, RSTRT = RFAR).
- RSTRT must be specified for IOPS = 1 and IOPS = 3 in order to implement the air-flow model.

- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 20.000.

DELR:

- DELR is a spatial increment in the horizontal direction that defines the frequency of pressure and flow output within the limits of RSTRT and RFAR (see figure 7). For IOPS = 1 and IOPS = 3, DELR represents the horizontal spacing between consecutive pressure and flow-output values. For IOPS = 2, DELR is not used because output is generated only along a vertical line.
- DELR must be specified for IOPS = 1 and IOPS =3 in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.00.

RFAR:

- RFAR is a spatial limit in the horizontal direction that defines the distance to the point farthest from the well for which pressure and flow output are generated (see Figure 6). The distance is relative to the center line of the well, and there is no limit on the maximum value that can be entered. For IOPS = 1 and IOPS = 3, RFAR represents the horizontal distance from the well centerline to the far limit of the pressure and flow output line and domain, respectively. For IOPS=2, RFAR represents the horizontal distance from the well centerline to the vertical line along which pressure and flow are output (for IOPS = 2, RSTRT = RFAR).
- RFAR must be specified to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 250.000.

DELZ:

- DELZ is a spatial increment in the vertical direction that defines the frequency of pressure and flow output within the limits of ZOBS and ZFAR (see figure 7). For IOPS = 2 and IOPS = 3, DELZ represents the vertical spacing between consecutive pressure and flow output values. For IOPS = 1, DELZ is not used because output is generated only along a horizontal line.
- DELZ must be specified for IOPS = 2 and IOPS = 3 in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 10.000.

ZFAR:

- ZFAR is a spatial limit in a vertical direction that defines the depth to a point farthest from either the land surface (for IOP2=1) or the lower limit of the upper unit (for IOP2=2 or IOP2=3) for which pressure and flow output are generated (see Figure 6). The maximum depth specified cannot exceed the depth of the domain (ZB). For IOPS = 2 and IOPS = 3, ZFAR represents the vertical distance from the land surface to the far limit of the pressure and flow output. For IOPS = 1, ZFAR is not used because the vertical distance to the output line is defined by ZOBS (for IOPS = 1, ZOBS = ZFAR).
- ZFAR must be specified for IOPS = 2 and IOPS = 3 in order to implement the air-flow model.
- Numeric input only is accepted (real).
- Units depend on IU1(1); default is cm.
- Input length cannot exceed 10 characters: (F10.3).
- Input example: 160.000.

4.5.2 Pressure Output File OPVSR

In the prediction mode, AIR2D calculates pressure and volumetric and mass specific discharges at specified radii and depths. This section describes the pressure output from AIR2D. If no filename is specified for pressure predictions, output is written to the file PVSR.CUT. Alternatively, the user can specify separate output filenames (stored as variable OPVSR in the TEST4xx input file) to record the pressure predictions. No option is available for viewing pressure predictions on the screen.

Pressure output will depend on the output option (IOPS) specified in the input file by the user (see Section 4.5.1). Examples of pressure output for each option will be presented, including:

1) output along a horizontal line (that is, IOPS = 1);

2) output along a vertical line (that is, IOPS = 2);

3) output in a vertical section (that is, IOPS = 3).

The spatial range of output values is shown in figure 7.

The units used in the output file depend on the values for length, volume, time, pressure, temperature, mass, and permeability specified in the input file (see Section 4.5.1). A record of the units used in the simulation is presented in the WELLx.OUT output file (see Section 4.5.5).

File specifications are shown below.

Name of file:	Specified by the user (for example, P11.OUT or PVSR.OUT (default)).
File contents:	Depth at which pressure applies, radial distance from well centerline at which pressure applies, pressure prediction for prevailing conditions.
File application:	This file is used to record pressure predictions in the model domain based on applications of the analytical air-flow equation.
File unit number:	The program defines the output file as UNIT = 14.

Program output:	Results are output from the subroutine POWELL. Output from the simulation is written for each well mass flow rate specified. If no filename is specified by the user and pressure distribution output is generated, data are directed to the file PVSR.OUT. Separate output filenames can be specified by the user (see Section 4.5.1). Output is not displayed on the screen.
Data units:	Data units are indicated in the WELL.OUT file. Units conform to the user's specifications. If no selections are made by the user, data is output in the default unit system.

An example of the file, pressure output for IOPS = 1, is given below.

```
--------------------------------------------
  Radial      Depth     Pressure along
 distance              horizontal line
   (cm)        (cm)        (atm)
--------------------------------------------
  20.00     -130.00      .937370E+00
  30.00     -130.00      .950624E+00
  40.00     -130.00      .958979E+00
  50.00     -130.00      .964758E+00
  60.00     -130.00      .968988E+00
  70.00     -130.00      .972213E+00
  80.00     -130.00      .974749E+00
  90.00     -130.00      .977208E+00
 100.00     -130.00      .978757E+00
 110.00     -130.00      .980079E+00
 120.00     -130.00      .981222E+00
 130.00     -130.00      .982220E+00
 140.00     -130.00      .983102E+00
 150.00     -130.00      .983886E+00
 160.00     -130.00      .984591E+00
 170.00     -130.00      .985229E+00
 180.00     -130.00      .985809E+00
 190.00     -130.00      .986341E+00
 200.00     -130.00      .986831E+00
 210.00     -130.00      .987285E+00
 220.00     -130.00      .987708E+00
 230.00     -130.00      .988103E+00
 240.00     -130.00      .988473E+00
 250.00     -130.00      .988822E+00
```

An example of the file, pressure output for IOPS = 2, is given below.

```
--------------------------------------------
 Radial       Depth     Pressure along
 distance              horizontal line
   (cm)        (cm)        (atm)
--------------------------------------------
 100.00     -100.00      .979605E+00
 100.00     -110.00      .979026E+00
 100.00     -120.00      .978627E+00
 100.00     -130.00      .978757E+00
 100.00     -140.00      .978514E+00
 100.00     -150.00      .978799E+00
 100.00     -160.00      .979265E+00
```

An example of the file, pressure output for IOPS = 3, is given below.

```
 Radial    Depth      Pressure along
distance              horizontal line
  (cm)       (cm)         (atm)

 20.00   -100.00      .953406E+00
 30.00   -100.00      .960581E+00
 40.00   -100.00      .965586E+00
 50.00   -100.00      .969342E+00
 60.00   -100.00      .972281E+00
 70.00   -100.00      .974637E+00
 80.00   -100.00      .976587E+00
 90.00   -100.00      .978219E+00
100.00   -100.00      .979605E+00
110.00   -100.00      .980799E+00
120.00   -100.00      .981839E+00
...........
220.00   -160.00      .987642E+00
230.00   -160.00      .988028E+00
240.00   -160.00      .988392E+00
250.00   -160.00      .988736E+00
```

4.5.3 Volumetric Specific-Discharge Output File OVVSR

In the prediction mode, AIR2D calculates pressure and volumetric and mass specific discharges at specified radii and depths. This section describes the volumetric specific-discharge output from AIR2D. If no filename is specified for the specific-discharge predictions, output is written to the file VVSR.OUT. Alternatively, the user can specify separate output filenames (stored as variable OVVSR in the TEST4xx input file) to record the volumetric specific-discharge predictions. No option is available for viewing flow predictions on the screen.

Volumetric specific-discharge output depends on the option (IOPS) specified in the input file by the user. Examples of volumetric specific-discharge output for each option are presented, including

(1) output along a horizontal line (that is, IOPS = 1),

(2) output along a vertical line (that is, IOPS = 2), and

(3) output in a vertical section (that is, IOPS = 3).

The spatial range of output values is shown in figure 7.

The units used in the output file depend on the values for length, volume, and time specified in the input file (see Section 4.5.1). A record of the units used in the simulation is presented in the WELLx.OUT output file (see Section 4.5.5).

File specifications are as follows:

Name of file: Specified by the user (for example, V11.OUT or VVSR.OUT (default)).
File contents: Depth of specific discharge, radial distance from well centerline to specific discharge, volumetric specific discharge in the horizontal direction, volumetric specific discharge in the vertical direction.
File application: This file is used to record volumetric specific-discharge predictions in the model domain based on applications of the analytical air-flow equation.
File unit number: The program defines the output file as UNIT = 15.
Program output: Results are output directly from the subroutine POWELL. Output from the simulation is written for each well mass flow rate specified. If no filename is specified by the user and volumetric specific-discharge output is generated, data are directed to the file VVSR.OUT. Separate output filenames can be specified by the user for the DIRECT entry mode (see Section 4.5.1). Output is not displayed on the screen.
Data units: Data units are indicated in the WELL.OUT file. Units conform to the user's specifications. If no selections are made by the user, data are output in the default unit system.

An example of volumetric specific discharge output for IOPS = 1 is given below.

```
  Radial     Depth      Horizontal        Vertical         Resultant
 distance               specific          specific         specific
                        discharge         discharge        discharge
   (cm)      (cm)      (cm^3/s/cm^2)     (cm^3/s/cm^2)    (cm^3/s/cm^2)

   20.00   -130.00    -.115375E+00     .180380E-03     -.115375E+00
   30.00   -130.00    -.663253E-01     .177567E-03     -.663256E-01
   40.00   -130.00    -.400139E-01     .175474E-03     -.400143E-01
   50.00   -130.00    -.286224E-01     .173699E-03     -.286229E-01
   60.00   -130.00    -.214452E-01     .172053E-03     -.214459E-01
   70.00   -130.00    -.166336E-01     .170441E-03     -.166345E-01
   80.00   -130.00    -.132616E-01     .168811E-03     -.132627E-01
   90.00   -130.00    -.108126E-01     .167061E-03     -.108139E-01
  100.00   -130.00    -.899367E-02     .165342E-03     -.899519E-02
  110.00   -130.00    -.760720E-02     .163547E-03     -.760896E-02
  120.00   -130.00    -.652977E-02     .161671E-03     -.653177E-02
  130.00   -130.00    -.567821E-02     .159720E-03     -.568046E-02
  140.00   -130.00    -.499499E-02     .157699E-03     -.499748E-02
  150.00   -130.00    -.443936E-02     .155612E-03     -.444208E-02
  160.00   -130.00    -.398189E-02     .153467E-03     -.398485E-02
  170.00   -130.00    -.355832E-02     .151270E-03     -.356153E-02
  180.00   -130.00    -.325115E-02     .149028E-03     -.325457E-02
  190.00   -130.00    -.298801E-02     .146747E-03     -.299161E-02
  200.00   -130.00    -.276088E-02     .144435E-03     -.276465E-02
  210.00   -130.00    -.256343E-02     .142099E-03     -.256736E-02
  220.00   -130.00    -.239060E-02     .139744E-03     -.239468E-02
  230.00   -130.00    -.223835E-02     .137377E-03     -.224256E-02
  240.00   -130.00    -.210338E-02     .135003E-03     -.210771E-02
  250.00   -130.00    -.198303E-02     .132628E-03     -.198746E-02
         VOLUMETRIC FLOW SIGN CONVENTION:
         NEGATIVE HORIZONTAL FLOW => FLOW TOWARDS WELL
         POSITIVE HORIZONTAL FLOW => FLOW AWAY FROM WELL
         NEGATIVE VERTICAL FLOW   => FLOW UPWARDS
         POSITIVE VERTICAL FLOW   => FLOW DOWNWARDS
```

An example of volumetric specific discharge output for IOPS = 2 is given below.

```
 Radial      Depth      Horizontal        Vertical         Resultant
distance                specific          specific         specific
                        discharge         discharge        discharge
  (cm)       (cm)      (cm^3/s/cm^2)     (cm^3/s/cm^2)    (cm^3/s/cm^2)

 100.00    -100.00    -.750830E-02      .190710E-02     -.774671E-02
 100.00    -110.00    -.832759E-02      .145739E-02     -.845416E-02
 100.00    -120.00    -.888419E-02      .857062E-03     -.892543E-02
 100.00    -130.00    -.899367E-02      .165342E-03     -.899519E-02
 100.00    -140.00    -.889130E-02     -.525844E-03     -.890684E-02
 100.00    -150.00    -.834179E-02     -.112484E-02     -.841728E-02
 100.00    -160.00    -.752954E-02     -.157228E-02     -.769194E-02


           VOLUMETRIC FLOW SIGN CONVENTION:
           ---------- ---- ---- ----------

           NEGATIVE HORIZONTAL FLOW => FLOW TOWARDS WELL
           POSITIVE HORIZONTAL FLOW => FLOW AWAY FROM WELL

           NEGATIVE VERTICAL FLOW   => FLOW UPWARDS
           POSITIVE VERTICAL FLOW   => FLOW DOWNWARDS
```

An example of volumetric specific discharge output for IOPS = 3 is shown below.

```
 Radial        Depth       Horizontal       Vertical        Resultant       Flow     No.
distance                   specific         specific        specific        angle
                           discharge        discharge       discharge
  (cm)         (cm)       (cm^3/s/cm^2)    (cm^3/s/cm^2)   (cm^3/s/cm^2)    (deg)    (-)

     20.00    -100.00    -.542812E-01    .326953E-01    .633675E-01    211.06    92
     30.00    -100.00    -.343571E-01    .190561E-01    .392880E-01    209.01    92
     40.00    -100.00    -.250970E-01    .121838E-01    .278981E-01    205.90    92
     50.00    -100.00    -.193038E-01    .826286E-02    .209979E-01    203.17    92
     60.00    -100.00    -.153493E-01    .584187E-02    .164234E-01    200.84    92
     70.00    -100.00    -.125056E-01    .424786E-02    .132074E-01    198.76    92
     80.00    -100.00    -.103878E-01    .318738E-02    .108658E-01    197.06    92
     90.00    -100.00    -.876971E-02    .244236E-02    .910346E-02    195.56    92
    100.00    -100.00    -.750830E-02    .190710E-02    .774671E-02    194.25    92
    110.00    -100.00    -.651025E-02    .151501E-02    .668420E-02    193.10    92
    120.00    -100.00    -.570505E-02    .122288E-02    .583464E-02    192.10    92
    130.00    -100.00    -.504955E-02    .100192E-02    .514799E-02    191.22    92
    140.00    -100.00    -.450961E-02    .832503E-03    .458581E-02    190.46    92
    150.00    -100.00    -.406014E-02    .701113E-03    .412023E-02    189.80    92
    160.00    -100.00    -.368229E-02    .598059E-03    .373054E-02    189.23    92
    170.00    -100.00    -.336177E-02    .516424E-03    .340120E-02    188.73    92
    180.00    -100.00    -.308755E-02    .451163E-03    .312034E-02    188.31    92
    190.00    -100.00    -.285107E-02    .398542E-03    .287879E-02    187.96    92
    200.00    -100.00    -.264578E-02    .355583E-03    .266957E-02    187.65    92
    210.00    -100.00    -.246589E-02    .320619E-03    .248664E-02    187.41    92
    220.00    -100.00    -.230742E-02    .291738E-03    .232579E-02    187.21    92
    230.00    -100.00    -.216694E-02    .267709E-03    .218341E-02    187.04    92
    240.00    -100.00    -.204165E-02    .247568E-03    .205660E-02    186.91    92
```

```
 .........
 .........
 210.00   -160.00   -.249442E-02   -.342024E-04    .249465E-02    179.21   92
 220.00   -160.00   -.233612E-02   -.101709E-04    .233615E-02    179.75   92
 230.00   -160.00   -.219574E-02    .897458E-05    .219576E-02    180.23   92
 240.00   -160.00   -.207047E-02    .242156E-04    .207061E-02    180.67   92
 250.00   -160.00   -.195805E-02    .363357E-04    .195839E-02    181.06   92
```

4.5.4 Mass Specific-Discharge Output File OMVSR

In the prediction mode, AIR2D calculates pressure and volumetric and mass specific discharges at specified radii and depths. This section describes the mass specific-discharge output from AIR2D. If no filename is specified for mass specific-discharge predictions, output is written to the file MVSR.OUT. Alternatively, the user can specify separate output filenames (stored as variable OMVSR in the TEST4xx input file) to record the mass specific-discharge predictions. No option is available for viewing predictions on the screen.

Mass specific-discharge output depends on the output option (IOPS) specified in the input file by the user (see Section 4.5.1). Examples of mass flow output for each option are presented, including

(1) output along a horizontal line (IOPS = 1),

(2) output along a vertical line (IOPS = 2), and

(3) output in a vertical section (IOPS = 3).

The spatial range of output values is shown in figure 7.

The units used in the output file depend on the values for length, time, and mass specified in the input file (see Section 4.5.1). A record of the units used in the simulation is presented in the WELLx.OUT output file (see Section 4.5.5).

File specifications are shown below.

Name of file:	Specified by the user (for example, M11.OUT or MVSR.OUT (default)).
File contents:	Depth to mass specific-discharge component, radial distance from well center line to mass specific-discharge component, mass specific-discharge in the horizontal direction, mass specific-discharge in the vertical direction.
File application:	This file is used to record mass specific-discharge predictions in the model domain based on applications of the analytical air-flow equation.
File unit number:	The program defines the output file as UNIT = 16.
Program output:	Output from the simulation is written for each well mass flow rate specified. If no filename is specified by the user and mass specific-discharge output is generated, data are directed to the file MVSR.OUT. Separate output filenames can be specified by the user for the DIRECT entry mode (see Section 4.5.1). Output is not displayed on the screen.
Data units:	Data units are indicated in the WELL.OUT file. Units conform to the user's specifications. If no selections are made by the user, data are output in the default unit system.

An example of mass specific-discharge output for IOPS = 1 is given below.

```
 Radial     Depth       Horizontal      Vertical        Resultant
distance                specific        specific        specific
                        discharge       discharge       discharge
  (cm)       (cm)       (g/s/cm^2)      (g/s/cm^2)      (g/s/cm2)

  20.00    -130.00    -.134055E-03     .209585E-06    -.134056E-03
  30.00    -130.00    -.781536E-04     .209234E-06    -.781539E-04
  40.00    -130.00    -.475643E-04     .208585E-06    -.475648E-04
  50.00    -130.00    -.342283E-04     .207720E-06    -.342289E-04
  60.00    -130.00    -.257578E-04     .206654E-06    -.257587E-04
  70.00    -130.00    -.200451E-04     .205398E-06    -.200462E-04
  80.00    -130.00    -.160233E-04     .203964E-06    -.160246E-04
  90.00    -130.00    -.130972E-04     .202359E-06    -.130988E-04
 100.00    -130.00    -.109112E-04     .200595E-06    -.109131E-04
 110.00    -130.00    -.924160E-05     .198684E-06    -.924374E-05
 120.00    -130.00    -.794193E-05     .196634E-06    -.794436E-05
 130.00    -130.00    -.691324E-05     .194459E-06    -.691597E-05
 140.00    -130.00    -.608687E-05     .192171E-06    -.608990E-05
 150.00    -130.00    -.541410E-05     .189780E-06    -.541742E-05
 160.00    -130.00    -.485966E-05     .187298E-06    -.486327E-05
 170.00    -130.00    -.434553E-05     .184736E-06    -.434945E-05
 180.00    -130.00    -.397275E-05     .182104E-06    -.397692E-05
 190.00    -130.00    -.365317E-05     .179415E-06    -.365757E-05
 200.00    -130.00    -.337716E-05     .176676E-06    -.338177E-05
 210.00    -130.00    -.313707E-05     .173898E-06    -.314189E-05
 220.00    -130.00    -.292683E-05     .171089E-06    -.293182E-05
 230.00    -130.00    -.274152E-05     .168258E-06    -.274668E-05
 240.00    -130.00    -.257717E-05     .165413E-06    -.258248E-05
 250.00    -130.00    -.243057E-05     .162561E-06    -.243600E-05


      MASS FLOW SIGN CONVENTION:
      ---- ---- ---- ----------

      NEGATIVE HORIZONTAL FLOW => FLOW TOWARDS WELL
      POSITIVE HORIZONTAL FLOW => FLOW AWAY FROM WELL

      NEGATIVE VERTICAL FLOW   => FLOW UPWARDS
      POSITIVE VERTICAL FLOW   => FLOW DOWNWARDS


      MASS FLOW SUMMARY:
      ---- ---- -------

      AT DEPTH   130.0000 cm BELOW THE SURFACE, AND
      BETWEEN RADII   20.0000 cm AND  250.0000 cm
      TOTAL VERTICAL FLOW OVER TWO PI RADIANS =    -.358846E-01   g/sec
      WHICH REPRESENTS  3.59% OF FLOW OUT OF WELL
```

An example of mass specific-discharge output for IOPS = 2 is given below.

```
 Radial     Depth      Horizontal         Vertical           Resultant
Distance               specific           specific           specific
                       discharge          discharge          discharge
  (cm)       (cm)      (g/s/cm^2)         (g/s/cm^2)         (g/s/cm2)

 100.00    -100.00    -.911703E-05        .231572E-05      -.940653E-05
 100.00    -110.00    -.101059E-04        .176860E-05      -.102595E-04
 100.00    -120.00    -.107770E-04        .103966E-05      -.108270E-04
 100.00    -130.00    -.109112E-04        .200595E-06      -.109131E-04
 100.00    -140.00    -.107843E-04       -.637801E-06      -.108032E-04
 100.00    -150.00    -.101208E-04       -.136473E-05      -.102124E-04
 100.00    -160.00    -.913965E-05       -.190850E-05      -.933678E-05

            MASS FLOW SIGN CONVENTION:
            ---- ---- ---- ----------

            NEGATIVE HORIZONTAL FLOW => FLOW TOWARDS WELL
            POSITIVE HORIZONTAL FLOW => FLOW AWAY FROM WELL

            NEGATIVE VERTICAL FLOW   => FLOW UPWARDS
            POSITIVE VERTICAL FLOW   => FLOW DOWNWARDS

            MASS FLOW SUMMARY:
            ---- ---- -------

            AT RADIUS   100.0000 cm FROM THE WELL CENTER LINE, AND,
            BETWEEN DEPTHS   100.0000 cm AND   160.0000 cm
            TOTAL HORIZONTAL FLOW OVER TWO PI RADIANS =    -.388836E+00  g/s
            WHICH REPRESENTS 38.88% OF FLOW OUT OF WELL
```

An example mass specific-discharge output for IOPS = 3 is given below.

```
  Radial     Depth      Horizontal        Vertical          Resultant        Flow    No.
 distance               specific          specific          specific         angle
                        discharge         discharge         discharge
   (cm)       (cm)      (g/s/cm^2)        (g/s/cm^2)        (g/s/cm^2)       (deg)   (-)

    20.00   -100.00    -.641489E-04      .386388E-04      .748868E-04      211.06    92
    30.00   -100.00    -.409083E-04      .226897E-04      .467794E-04      209.01    92
    40.00   -100.00    -.300382E-04      .145826E-04      .333908E-04      205.90    92
    50.00   -100.00    -.231943E-04      .992816E-05      .252298E-04      203.17    92
    60.00   -100.00    -.184987E-04      .704052E-05      .197932E-04      200.84    92
    70.00   -100.00    -.151081E-04      .513185E-05      .159559E-04      198.76    92
    80.00   -100.00    -.125746E-04      .385839E-05      .131532E-04      197.06    92
    90.00   -100.00    -.106336E-04      .296147E-05      .110383E-04      195.56    92
   100.00   -100.00    -.911703E-05      .231572E-05      .940653E-05      194.25    92
   110.00   -100.00    -.791477E-05      .184186E-05      .812626E-05      193.10    92
   120.00   -100.00    -.694322E-05      .148828E-05      .710094E-05      192.10    92
   130.00   -100.00    -.615117E-05      .122050E-05      .627108E-05      191.22    92
   140.00   -100.00    -.549800E-05      .101497E-05      .559090E-05      190.46    92
   150.00   -100.00    -.495369E-05      .855414E-06      .502700E-05      189.80    92
   160.00   -100.00    -.449570E-05      .730169E-06      .455461E-05      189.23    92
   170.00   -100.00    -.410688E-05      .630886E-06      .415506E-05      188.73    92
   180.00   -100.00    -.377399E-05      .551467E-06      .381407E-05      188.31    92
```

```
 . . . . . . . . . .
 . . . . . . . . . .
 210.00   -160.00   -.305245E-05   -.418539E-07    .305274E-05    179.21   92
 220.00   -160.00   -.285994E-05   -.124514E-07    .285996E-05    179.75   92
 230.00   -160.00   -.268913E-05    .109912E-07    .268915E-05    180.23   92
 240.00   -160.00   -.253665E-05    .296679E-07    .253682E-05    180.67   92
 250.00   -160.00   -.239975E-05    .445322E-07    .240016E-05    181.06   92
```

4.5.5 Well Output File WELL.OUT

An additional file, WELL.OUT, records pressure and flow at the well, as generated by AIR2D. The user specifies the mass flow rate at the well as an input value. The model then calculates pressure at the well. The calculated pressure at the well is used to determine the density of the air in the well. By calculating the quotient of mass flow and air density, an estimate of the volumetric flow through the well is obtained. If no filename is specified for well output, pressure and flow at the well are written to the file WELL.OUT. Alternatively, the user can specify separate output filenames (stored as variable OWELL in the TEST4xx input file) to record the well output predictions. No option is available for viewing well pressure and flow predictions on the screen. The information written to the output file includes

(1) pressure in the well (in input units),

(2) volumetric flow rate (in input units), and

(3) mass flow rate (in input units).

The units used in the output file depend on the values for length, volume, time, pressure, temperature, mass, and permeability specified in the input file (see Section 4.5.1). A record of the units used in the simulation is included in the WELLx.OUT output file.

Output is written to the well output file once per simulation. No option is available for viewing the output on the screen.

An example of the well and unit summary IOPS = 1 is given below.

```
MID-DEPTH OF WELL FROM SURFACE  = -130.000 cm
RADIUS OF FILTER-SOIL INTERFACE =   10.001 cm
PRESSURE IN WELL                =     .912 atm
VOLUMETRIC FLOW THROUGH WELL    =   -.8848E+03 cm^3/sec

MASS FLOW THROUGH WELL          =   -1.000  g/sec

POSITIVE REPRESENTS INJECTION
NEGATIVE REPRESENTS WITHDRAWAL

SUMMARY OF UNITS USED IN SIMULATION
LENGTH UNIT SYSTEM    :  cm
VOLUME UNIT SYSTEM    :  cm^3
TIME UNIT SYSTEM      :  sec
PRESSURE UNIT SYSTEM  :  atm
TEMPERATURE UNIT SYSTEM:  degC
MASS UNIT SYSTEM      :   g
PERMEABILITY UNIT SYSTEM:  cm^2
```

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