DOCUMENTATION OF AIR3D, AN ADAPTATION OF THE GROUND-WATER-FLOW CODE MODFLOW TO SIMULATE THREE-DIMENSIONAL AIR FLOW IN THE UNSATURATED ZONE

By Craig J. Joss and Arthur L. Baehr

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BRUCE BABBITT, *Secretary*

U.S. GEOLOGICAL SURVEY

Gordon P. Eaton, *Director*

For additional information
write to:

District Chief
U.S. Geological Survey
810 Bear Tavern Road
Suite 206
West Trenton, NJ 08628

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REFERENCES

ATTACHMENTS

In pocket--Diskette containing the following files in each of two directories MAIN and PC:

- An instructional narrative file
- Fortran source file for preprocessor PREAIR
- Fortran source file for postprocessor POSTAIR
- Example input files for PREAIR and POSTAIR
- Fortran source files for MODFLOW package

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 AIR3D, AN ADAPTATION OF THE GROUND-WATER-FLOW CODE MODFLOW TO SIMULATE THREE-DIMENSIONAL AIR FLOW IN THE UNSATURATED ZONE

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ABSTRACT

This report documents a sequence of computer codes, called AIR3D, which adapt the ground-water-flow simulator MODFLOW (McDonald, M.G, and Harbaugh, A.L., 1988, A modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations, book 6, chap. A1, 586 p.) to simulate air flow in the unsaturated zone. This software package can be used to simulate three-dimensional air flow in a heterogeneous, anisotropic, unsaturated domain where air flow is induced through dry wells or trenches, as in vapor-extraction remediation. Although the code was developed primarily for this purpose, it also can be used to simulate natural air flow in the unsaturated zone caused by atmospheric-pressure variations. In this application, elevation-head and temperature-gradient terms are assumed to be negligible compared to pressure-gradient terms; therefore, AIR3D may not be appropriate for simulating natural flows in deep unsaturated systems.

A preprocessor (PREAIR) uses pneumatic and geologic information to create data files in a format consistent with MODFLOW input requirements. MODFLOW can be used to numerically solve the partial-differential equation governing air flow because the air-flow equation has been cast in a format consistent with the ground-water-flow equation. A postprocessor (POSTAIR) then transforms output from MODFLOW into dimensionally consistent air-flow output--pressure, mass flow rates, and volumetric flow rates.

MODFLOW is adapted by matching coefficients of the general, three-dimensional, transient air-flow equation with those of the ground-water-flow equation. The application of boundary conditions for air flow is facilitated by AIR3D. The approach retains the original MODFLOW features that permit solution of a model describing three-dimensional flow in heterogenous, anisotropic domains.

The preprocessor PREAIR and postprocessor POSTAIR are written in Fortran 77 and will run, with minor modification, on most computers with a Fortran compiler. PREAIR, MODFLOW, and POSTAIR exchange text and binary-data files and, therefore, all must be compiled with the same compiler.

SECTION 1--INTRODUCTION AND USER'S GUIDE

The solution of problems involving the movement of air in the unsaturated zone requires simulation of flow over a wide range of field conditions. For example, vapor extraction is emerging as a successful technology for remediating gasoline-contaminated unsaturated zones. Although this method, in which wells screened in the unsaturated zone are pumped to induce air flow, is conceptually straight forward, flow paths can be complex as a result of the effects of sediment layering, moisture variation, multiple well locations, and boundaries such as surface structures and pavement. Because the performance of a vapor-extraction system depends directly on the flow of air intersecting the contaminant plume, a mathematical model capable of simulating induced air flow would be a useful tool for placing and sizing wells.

Simulating air flow in porous media is conceptually equivalent to simulating ground-water flow. The U.S. Geological Survey (USGS) numerical ground-water-flow simulator MODFLOW, developed by McDonald and Harbaugh (1988), is widely used to simulate three-dimensional ground-water flow. The popularity of this code is the result of its ability to incorporate variable geologic conditions, its clearly defined input and output packages, and its successful menu of matrix solvers.

This report was prepared as part of the USGS Toxic Substances Hydrology Program and with the assistance of the Office of Ground Water. It documents the software package called AIR3D, which adapts MODFLOW to simulate air flow in the unsaturated zone. It includes a diskette containing all of the computer codes required to execute an air-flow simulation. Although it was developed primarily for simulating vapor extraction, AIR3D also may be useful in the simulation of natural air flow in the unsaturated zone caused by variations in atmospheric pressure. In this application, elevation-head and temperature-gradient terms are assumed to be negligible compared to pressure-gradient terms; therefore, AIR3D may not be appropriate for simulating natural flows in deep unsaturated systems. The user is referred to Baehr and Hult (1991) to determine the significance of neglecting elevation-head and temperature-gradient terms.

AIR3D accounts for differences between air flow and ground-water flow. In MODFLOW, fluid compressibility is assumed to be negligible; in AIR3D, however, air compressibility is modeled according to the ideal-gas law. The resulting nonlinear air-flow equation in terms of air pressure is linearized by expressing it in terms of air pressure squared (Section 2.1), as suggested by Muskat and Botset (1931) for modeling gas reservoirs. Because air is compressible, AIR3D computes and records both volumetric and mass flow rates (see Section 4.1). Also, to circumvent the problem of nonlinear boundary conditions arising from air compressibility, wells and trenches in the domain are modeled as constant-pressure cells in AIR3D and the implied mass flux is computed and recorded to an output file.

AIR3D takes advantage of the facility and computational power of MODFLOW by transforming the air-flow equation into a form equivalent to the ground-water-flow equation solved by MODFLOW (see Sections 2.1-2.2). This transformation, as well as data input for the simulation, is accomplished with the preprocessor Fortran program called PREAIR. Output files from PREAIR are input files to MODFLOW. MODFLOW then is invoked to solve numerically the three-dimensional air-flow equation. No changes in MODFLOW programs are required unless the user wishes to change the dimension of arrays. Output from MODFLOW is transformed by the postprocessor Fortran program called POSTAIR to interpret the simulation (see Section 2.3). Figure 1 illustrates the logic of the AIR3D package. The only files required from the user are INFILEx.PRE (Section 3.3.3), DATAIR.PRE (Section 3.3.4), and INFILEx.POS (Section 4.5.3). All other files are created in the required order by executing the programs PREAIR, MODFLOW, and POSTAIR in sequence.

Referring to figure 1, users familiar with MODFLOW will note that MODFLOW input files are generated only for the Basic Package (BASAIR), the Output-Control Package (OCAIR), the Block-Centered-Flow Package (BCFAIR), and either the SIP or the SOR Package (SIPAIR). The River, Recharge, Well, Drain, General-Head-Boundary, and Evapotranspiration Packages are not relevant for air-flow simulation. Also, the ground-water options for confined or unconfined layers or combinations thereof do not apply to air-flow cell layers, as cell layers are always saturated by air and, therefore, all cell- layer settings are defaulted to the confined designation. As a result of these simplifications, AIR3D simulations are easier to implement than general MODFLOW applications. The suffix AIR used in the diagram does not indicate an alteration in a MODFLOW subroutine; it is used merely to identify logic in the overall AIR3D package.

In the case of the matrix-solver option SIPAIR, only the Strongly Implicit Procedure (SIP) option and the Slice-Successive Overrelaxation Procedure (SOR) option presented by McDonald and Harbaugh (1988) have been evaluated for air-flow simulations and are included in AIR3D. Most AIR3D testing to date (1994) has employed SIP, and the performance of this option has been satisfactory. Future users, however, may perform simulations that can be executed more efficiently with a different matrix solver. The Preconditioned Conjugate Gradient matrix-solver option (PCG2) developed by Hill (1990) as an alternative to SIP and SOR may result in more numerically efficient AIR3D simulations. This option can be implemented in the AIR3D package by using the PCG2 subroutine and making the minor alterations to MODFLOW code given in Hill (1990).

The diskette provided with this document contains the following files in each of two directories MAIN and PC:

READ.ME--an instructional narrative (ASCII text file);

PREAIR.Fxx--preprocessor Fortran source code;

POSTAIR.Fxx--postprocessor Fortran source code;

MODFLOW.Fxx, BAS1.Fxx, BCF1.Fxx, DRN1.Fxx, EVT1.Fxx, GHB1.Fxx, RCH1.Fxx, RIV1.Fxx, SIP1.Fxx, SOR1.Fxx, UTL1.Fxx, and WEL1.Fxx--Fortran source codes for the MODFLOW package.

INFILE4.PRE, DATAIR4.PRE, and INFILE4.POS--example input files described in Sections 3.3.3 3.3.4, and 4.5.3.

The AIR3D Software Package

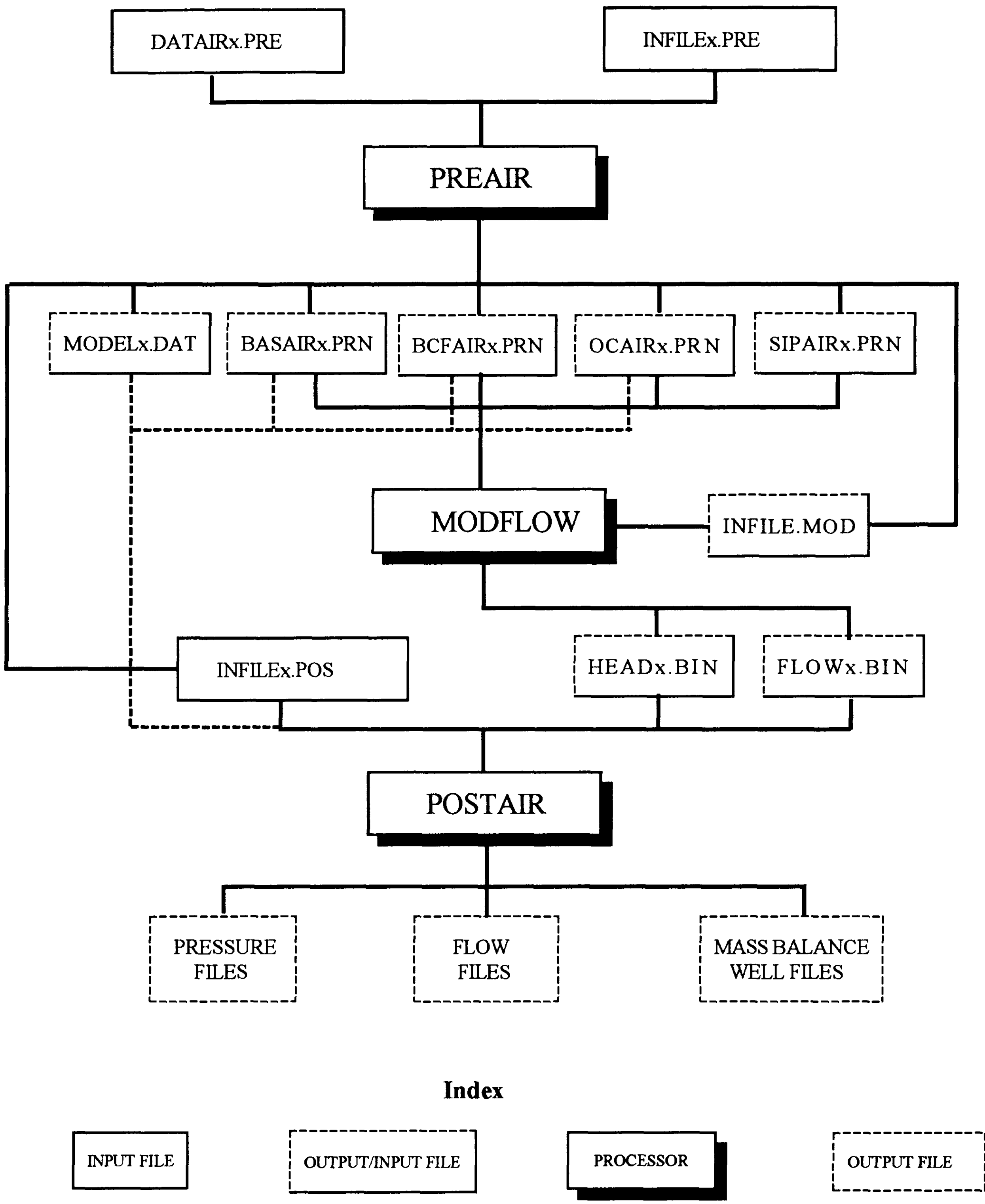

Figure 1.--The components of the AIR3D software package

The directory MAIN contains the files to be used on a mainframe computer. Default settings are specified accordingly and the Fortran codes have the extension F77 (eg. PREAIR.F77, POSTAIR.F77, etc.). The directory PC contains the files to be used on a personal computer. Default settings are specified accordingly and the Fortran codes have the extension FOR (eg. PREAIR.FOR, POSTAIR.FOR, etc.).

It is assumed that users have access to a Fortran compiler. The installation and execution procedure is as follows:

1. Copy files from diskette into a directory on your computer.
   Copy files from directory MAIN on the diskette if you are using a mainframe computer.
   Copy files from directory PC on the diskette if you are using a personal computer.

2. Check default settings.
   If your Fortran compiler requires an extension for Fortran code files other than .F77 or .FOR then rename the files accordingly. You may need to change the input and output unit number settings in PREAIR.Fxx, POSTAIR.Fxx, and MODFLOW.Fxx for compatibility with your computer. The sections of code defining these units are clearly identified in the source codes and also are defined in Section 3.2.1 for PREAIR.Fxx and in 4.2.1 for POSTAIR.Fxx.

3. Compile and load the source codes.
   For example the sequenceof commands for a Microsoft[1] Fortran compiler are as follows:

   ```
   FL PREAIR.FOR

   FL MODFLOW.FOR BAS1.FOR BCF1.FOR SIP1.FOR SOR1.FOR UTL1.FOR
         DRN1.FOR EVT1.FOR GHB1.FOR RCH1.FOR RIV1.FOR WEL1.FOR

   FL POSTAIR.FOR
   ```

4. Create three input files.
   Three input files are required to perform an AIR3D simulation, two for the preprocessor PREAIR to define the simulation and one for the postprocesser POSTAIR to define the organization of output. The input files for PREAIR may be created by running PREAIR and accessing the menu. They are defined as follows:

   INFILEx.PRE--(see Section 3.3.3)
   DATAIR.PRE--(see Section 3.3.4)

   The input file for POSTAIR may be created by running POSTAIR and accessing the menu, it is defined as follows:

   INFILEx.POS--(see Section 4.5.3).

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

5. Execute the programs PREAIR, MODFLOW, and POSTAIR in series.
For example, the sequence of commands for a personal computer are:

PREAIR--(see Section 3.2.3)
MODFLOW < INFILE.MOD
POSTAIR--(see Section 4.2.3),

Test simulations for AIR3D that match the numerical finite-difference solution against analytical solutions are defined in Section 5. It is helpful for users to test their understanding of the AIR3D software package by performing one of the test simulations.

SECTION 2.0--SIMULATION OF AIR ADVECTION IN THE UNSATURATED ZONE

2.1 Derivation of the Three-Dimensional Air-Flow Equation

The conservation-of-mass equation for air flow in an unsaturated porous medium is

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

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:

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

where, for the air phase in the unsaturated zone,

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

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-cm^2/s^2-mol-K]
T	= temperature	[K]

The elevation head in equation (3) is neglected so that all terms of the air-flow equation solved with AIR3D can be matched with the ground-water-flow equation solved with MODFLOW. Baehr and Hult (1991) demonstrate that, for induced flows associated with vapor extraction, this assumption is appropriate. Neglecting the elevation head in equation (3) may not be valid for natural flows in deep unsaturated zones induced by atmospheric-pressure variations. For this type of application, the user should test AIR3D against a one-dimensional (vertical) analytical solution for a homogeneous domain the same length as the heterogeneous natural system requiring numerical solution. Baehr and Hult (1991) also demonstrate that terms in the air-flow equation that arise as a result of variations in subsurface temperature can be neglected for induced flows; however, the importance of these terms for natural flow conditions has not been evaluated.

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

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

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

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

the following three-dimensional air-flow equation, in Cartesian coordinates results:

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

where x, y, and z are Cartesian coordinates. It is assumed that the coordinates are aligned with the major axes of the permeability tensor; therefore, k_{xx}, k_{yy}, and k_{zz} are the air permeabilities in the x, y, and z directions, respectively. Equation (7) is of the same form as the ground-water-flow equation solved with MODFLOW. Baehr and Hult (1991) present details involving the derivation of an air-flow equation in radial coordinates that illustrate the algebraic manipulations required to obtain equation (7).

Air-phase permeability is assumed to be independent of air-phase pressure P; therefore, the Klinkenberg slip effect (Klinkenberg, 1941) can only be modeled as constant with respect to P. Baehr and Hult (1991) examined the implications of this assumption for induced flow and concluded that it is valid over a wide range of conditions that are anticipated for vapor-extraction practice.

The coefficient S_a is the pneumatic equivalent of specific storage and, if air-filled porosity is constant with respect to time (that is, water movement is neglected), then:

$$S_a = \frac{\theta \mu}{(\phi)^{1/2}} \qquad (8)$$

The change of variable $\phi = P^2$ results in a linear equation for steady- state air flow because the term defined by equation (8) factors out. For transient air flow, equation (7) is linearized by means of the assumption that $\phi^{1/2} = P_{atm}$ in the definition of S_a above, where P_{atm} is the prevailing atmospheric pressure. This assumption, first suggested in the gas-reservoir- engineering literature, was used by Weeks (1978) in the transient analysis of natural vertical air movement in the unsaturated zone and was found to be appropriate for the transient analysis of induced air flow by Baehr and Hult (1988).

2.2 Interpretation of MODFLOW Ground-Water-Flow Equation

The following ground-water-flow equation is solved with MODFLOW (McDonald and Harbaugh, 1988):

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

where

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

h	= hydraulic head	[cm]
W	= volumetric flow per unit volume (hydraulic sources/sinks)	[s^{-1}]
S_S	= specific storage	[cm^{-1}]
t	= time	[s]

AIR3D simulates air flow by matching equations (7) and (9) so that the finite-difference numerical solution coded in MODFLOW can be used to solve the air-flow equation. This match is accomplished by replacing the following variables in MODFLOW with AIR3D parameters:

$$h \text{ is replaced by } \phi \tag{10}$$
$$K \text{ is replaced by } k \tag{11}$$
$$S_s \text{ is replaced by } S_a \tag{12}$$

2.3 Interpretation of MODFLOW output

MODFLOW simulation results are in terms of simulated heads and flows between adjacent cells. These values are converted to values of air pressure, volumetric flow, and mass flow through the unsaturated zone.

2.3.1 Interpretation of MODFLOW Head Output

As a result of the parameter matches discussed in the previous section, cell-by-cell values of ϕ are stored in the head-output file of MODFLOW for an air-flow simulation. Taking the square root of the head-output values yields the pressure distribution for the air-flow simulation. This calculation is implemented by the air-flow postprocessor, POSTAIR, discussed in Section 4.1.1.

2.3.2 Interpretation of MODFLOW Flow Output

MODFLOW stores cell-by-cell components of flow vectors, which need to be interpreted to obtain air-flow rates. Because air is compressible, air flow is specified as either a volumetric flow or a mass flow. MODFLOW calculates flow rates by using a finite-difference approximation for the following equation:

$$Q = -K A \frac{\partial h}{\partial l} \tag{13}$$

where

Q	= volumetric flow of water through cell in the l-direction	[cm^3/s]
K	= hydraulic conductivity	[cm/s]
A	= cross-sectional area of cell	[cm^2]
l	= length of cell	[cm]
h	= hydraulic-head	[cm]

On the basis of the transformations given by equations (10) and (11), flow output corresponds to the following terms for an AIR3D simulation:

$$Q^* = -k A \frac{\partial \phi}{\partial l} \tag{14}$$

where Q^* is an output related to (but not exactly) air flow in the units g^2-cm/s^4.

To relate Q^* to air flow, recognize that:

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

By substituting equation (15) into (14):

$$Q^* = 2\,k\,A\,P\,\frac{\partial P}{\partial l} \qquad (16)$$

From equation (5), Darcy's Law for volumetric air flow is as follows:

$$Q_v = \frac{k\,A}{\mu}\,\frac{\partial P}{\partial l} \qquad (17)$$

where

Q_v = volumetric-air-flow output term in the l-direction [cm^3/s]

MODFLOW flow output Q^* is converted as follows:

$$Q_v = Q^*\left(\frac{1}{2\,\mu\sqrt{\phi}}\right) \qquad (18)$$

Thus, to obtain components of volumetric air flow, the head-output file from MODFLOW must be combined with the MODFLOW flow-output file as indicated by equations (16) through (18).

Mass-air-flow rate is given by:

$$Q_m = \rho\,Q_v \qquad (19)$$

where

Q_m = mass air flow [g/s]

By substituting the ideal-gas law, as defined by equation (4), into equation (19), and then substituting into equation (17):

$$Q_m = - k A P \frac{\omega}{\mu R T} \frac{\partial P}{\partial l} \qquad (20)$$

Consequently, Q_m is given as follows:

$$Q_m = Q^* \left(\frac{\omega}{2 \mu R T} \right) \qquad (21)$$

Therefore, to obtain volumetric air flow, the MODFLOW flow-output file containing values for Q^* is multiplied by the factor that appears in equation (18) and, to obtain mass air flow, the MODFLOW flow-output file containing values for Q^* is multiplied by the factor that appears in equation (21).

SECTION 3.0--PREAIR PREPROCESSOR TO ADAPT MODFLOW FOR AIR-FLOW SIMULATIONS

The preprocessor Fortran code, PREAIR, defines data files for performing air-flow simulations with the U.S. Geological Survey three-dimensional, finite-difference ground-water-flow code MODFLOW. The preprocessor accepts geologic and air-flow information that describes the physical conditions to be modeled and generates data files for direct input into MODFLOW.

3.1 PREAIR Functions

The major functions of the air-flow preprocessor are to:

- substitute pneumatic parameters for the hydraulic parameters in MODFLOW (Section 3.1.1)
- specify initial conditions corresponding to the air-flow equation (Section 3.1.2)
- specify boundary conditions consistent with the air-flow model (Section 3.1.3)
- discretize the domain and assign parameter values to the cells (Section 3.1.4).

Four input files are required to use MODFLOW to simulate air flow simulations:

- a Basic File (Section 3.3.5)
- an Output-Control File (Section 3.3.6)
- a Block-Centered-Flow File (Section 3.3.7)
- a Matrix-Solver File (Section 3.3.8).

In addition, the preprocessor records information to a file called MODEL.DAT (see Section 3.3.10). This file is required by the postprocessor, POSTAIR, to interpret and organize the air-flow output. The postprocessor also requires an input file (for example, INFILEx.POS) that contains file names for pneumatic input. The preprocessor creates a default INFILEx.POS file that can be modified where necessary by using the interactive menu option in the postprocessor. Finally, the preprocessor creates a file called INFILEx.MOD, which records the names of the files required by MODFLOW.

3.1.1 Substitution of Variables

MODFLOW is a ground-water-flow model. The parameter definitions in MODFLOW, therefore, pertain to hydraulic properties of an aquifer. Certain variables must be substituted to simulate air flow through the unsaturated zone. A discussion of the required substitutions and their theoretical basis is presented in Section 2.2. These transformations include:

- replacing head values with values of air pressure squared
- replacing hydraulic conductivities with air-phase permeabilities
- replacing hydraulic storage coefficients with pneumatic equivalents.

The initial conditions ($\phi = P^2$ at $t = 0$) appear in the MODFLOW Basic input file in the Shead(NCOL,NROW) array (see Section 3.3.5). The air-flow equivalent to transmissivity appears in the MODFLOW Block-Centered-Flow input file in the Tran(NCOL,NROW) array (see Section 3.3.7). Note that, as with hydraulic conductivities, the air-phase permeabilities must be multiplied by the respective layer thicknesses to arrive at equivalent transmissivity terms. The preprocessor performs this operation. The storage coefficient appears in the MODFLOW Block-Centered-Flow input file in the sf1(NCOL,NROW) array (Section 3.3.7).

3.1.2 Initial Conditions for Air-Flow Simulations

The preprocessor assumes that the entire domain (except for cells that represent wells and trenches) is at atmospheric pressure at the start of the simulation; hence, the initial condition is a cell designation equal to the square of the prevailing atmospheric pressure. The user enters pressure in the selected unit system and the preprocessor converts pressure to units of centimeter-gram-second (cgs), according to:

1 atm = 760 mmHg at 0°C = 406.794 in. H_2O at 32°F = 101.325 kPa = 14.696 lb/in^2
= 1,013,250 g/cm-s^2

Hence, the head values at the start of the simulation that appear in the MODFLOW Basic-input-file array Shead(NCOL,NROW), for a prevailing pressure of 1 atmosphere, are defaulted to:

$$[1 \text{ atm}]^2 = 1.02668 \times 10^{12} \ (\text{g/cm-s}^2)^2$$

3.1.3 Boundary conditions for air-flow simulations

The boundary conditions imposed on the model domain by the air-flow preprocessor are as follows:

- an additional layer of cells is added above the uppermost model layer specified by the user, and a constant pressure of $\phi = P_{atm}^2$ is assigned to each cell, where P_{atm} is the prevailing atmospheric pressure in g/cm-s^2);
- lateral boundary cells in each layer are assigned a constant pressure of $\phi = P_{atm}^2$ to simulate lateral recharge from the surrounding unsaturated zone;
- cells in the lowest layer are assigned no flow, which represents an impervious water-table or confining-unit boundary;
- well and trench cells are assigned the square of a user-specified constant pressure.

The above specifications are set in the MODFLOW Basic input file in the IBOUND(NCOL,NROW) array (see Section 3.3.5). The reason for the boundary specifications is that recharge of air to the model domain ultimately must come from the atmosphere. This recharge can occur as direct leakage from the atmosphere (that is, from the additional layer of constant-pressure cells superimposed on the model by the preprocessor) or as leakage from the surrounding unsaturated zone (that is, from the constant-pressure lateral boundary cells specified within each cell layer). Note that, because AIR3D is a numerical model, lateral boundaries must be specified, even if the modeler's intention is to simulate a semi-infinite domain. Model output includes mass- balance calculations across the top and lateral boundaries, allowing the user to determine whether the lateral extent of the domain is sufficiently large. For example, in the case of vapor extraction, the user may be satisfied if 90 percent of the air entered the domain at the top boundary and 10 percent entered the domain at the lateral boundary.

The well (and trench) specification of constant pressure is chosen because conservation of mass for air, a compressible fluid, is not satisfied by specifying a volumetric flow rate distributed across the well (trench). Specification of mass-flow rate at the well or trench would ensure adherence to the conservation-of-mass principle; however, this option would introduce a nonlinear boundary condition and preclude the use of MODFLOW as a numerical solver. The nonlinear boundary condition would arise because mass flow is defined by the product of air density, given by equation (4), and volumetric flow (Darcy's Law), given by equation (5). Further, in the case of a well that intersects several layers, mass flow into the well from each layer varies according to, among other factors, the layer air permeability. For both transient and steady-state simulations, the pressure in the well is assigned a user-specified constant with depth. The implied mass and volumetric flow rates are computed and output by the postprocessor at each cell in the domain, including the well/trench boundary cells. On the basis of this information, the user can change layer air permeabilities and conduct another simulation, repeating this process until simulated pressure and flow correspond to field data. For these reasons, the iterative approach outlined above is recommended for modeling the nonlinear well/trench boundary condition.

3.1.4 Domain Discretization

MODFLOW solves the three-dimensional flow equation by using a finite- difference technique. Therefore, the domain must be discretized into rows, columns, and layers. MODFLOW requires direct input of cell widths along rows (DELR) and cell widths along columns (DELC) in the Block-Centered-Flow file; however, no equivalent input exists for cell depths along layers. To determine three-dimensional spatial coordinates corresponding to the positions of the pneumatic output parameters, layer thickness must be specified in the preprocessor input files. This allows pressure and flow rates to be given in terms of distances along rows (that is, X-coordinates), columns (that is, Y-coordinates), and layers (that is, Z-coordinates) by the postprocessor.

The row and column widths are transferred between the pre- and postprocessor directly by using the MODFLOW Block-Centered-Flow file. Because no equivalent MODFLOW file with data on layer depths exists, the preprocessor uses the file MODEL.DAT to record the vertical discretization. The cell depths, reference elevation, and other model information are then transferred between the pre- and postprocessors by using the MODEL.DAT file (see Section 3.3.10).

Note that the model discretization specified by the user can be tested by comparing the air recharge to the domain from the atmosphere with that from the lateral boundaries (see mass-balance file, Section 4.5.14) A desirable criterion for spacing rows and columns is to ensure that at least 90 percent of the air recharge to the domain originates from the atmospheric layer. When the atmospheric-recharge component is less than 90 percent the lateral boundaries can be extended either by increasing the number of rows and columns or by increasing the size of the rows and columns.

3.1.5 PREAIR Operations

PREAIR defines four input files for use with MODFLOW as well as three input files for recording, transferring, and entering data. The MODFLOW files include the Basic file, the Output-Control (OC) file, the Block-Centered-Flow (BCF) file, and the matrix-solver file (Strongly Implicit (SIP) or Successive Overrelaxation (SOR)). The remaining MODFLOW packages are not used for air-flow simulations and are defaulted to appropriate values by the preprocessor. MODFLOW file names are recorded to a file called INFILE.MOD by the preprocessor. Fortran input/output unit selections, physical parameters, layer depths, and well/trench information are transferred from the preprocessor to the postprocessor through a data file named MODEL.DAT. Finally, file names and default settings used in the postprocessor are written to an input file (for example, INFILEx.POS). General operations performed within the preprocessor are summarized below.

To produce the Basic file, the preprocessor performs the following operations:

- convert input units to the cgs unit system
- increase the number of geologic layers by one to account for the superimposed atmospheric layer
- set time units to seconds (ITMUNI=1)
- set Fortran unit numbers for the OC, BCF, and SIP or SOR files
- set Fortran unit numbers for the WEL, DRN, RIV, EVT, GHB, and RCH files to zero
- set IAPART = 0 and ISTRT = 0
- set boundary array (IBOUND) with a superimposed atmospheric layer, boundary cells, and well/trench cells for screened intervals specified as constant- pressure cells, cells located in unscreened well/trench casing set to inactive cells and remaining cells set to active
- set HNOFLO = 0.1027×10^{19} (this causes pressure output to appear as 1,000 atm for inactive cells)
- starting heads in all cells are assigned the prevailing atmospheric pressure squared in cgs units (for example, for 1 atm, starting heads are set at 1.2668×10^{12} $(g/cm\text{-}s^2)^2$) except for wells and trench cells, where starting heads are set at the applied vacuum/pressure squared.

The settings in the Basic file not specifically listed above are input according to standard MODFLOW requirements.

For the Output-Control file, the preprocessor defaults all of the settings as follows:

- IHEDFM = 0, IDDNFM = 0, IHEDUN = 12, IDDNUN = 0
- INCODE = 0, IHDDFL = 1, IBUDFL = 0, ICBCFL = 1
- Hdpr = 0, Ddpr = 0, Hdsv = 1, Ddsv = 0.

The above settings allow the necessary binary files containing pressure and flow-rate output to be generated by MODFLOW. Note that no binary files are generated for pressure differential (drawdown) with the preprocessor defaults. If drawdown output is required, set IDDNUN = 14 and Ddsv = 1 and recompile the program. Information written to the text output file by MODFLOW is kept to a minimum because the values have not undergone the necessary transformations to make them compatible with the air-flow parameters and are, therefore, of little value.

For the Block-Centered-Flow file, the preprocessor performs the following operations:

- set IBCFCB = 13
- set LAYCON(I) = 0 for each layer, because layers are treated as being confined
- note that no input values are required in air-flow simulations for arrays HY(NCOL,NROW), BOT(NCOL,NROW), sf2(NCOL,NROW), TOP(NCOL,NROW)
- set, for transient simulations, sf1(NCOL,NROW) = (air phase porosity)*(cell depth)*(air viscosity)/(atmospheric pressure)
- set Tran(NCOL,NROW) = (horizontal, intrinsic air phase permeability along rows)*(cell depth)
- set Vcont(NCOL,NROW) = (vertical air phase permeability along layers)/(cell depth).

For the superimposed atmospheric layer, parameters are set as follows: TRPY(1) = 1.0, sf1(NCOL,NROW) = 1.0, and Tran(NCOL,NROW) = 1.0. A value must be assigned for Vcont(NCOL,NROW) for the superimposed atmospheric layer. The default (recommended) value is obtained by setting Vcont(NCOL,NROW) equal to 100 times the vertical permeability in the uppermost geologic layer specified by the user divided by 0.2 times the depth of the cells in that layer. This default value was chosen to ensure that flow is not impeded in the superimposed atmospheric layer, while maintaining relevance to the rest of the domain descretization. This default specification will prevent the numerical difficulties associated with sharp discontinuity in the Vcont parameter. Alternatively, the value assigned to Vcont(NCOL,NROW) for the superimposed atmospheric layer can be specified by the user. The parameters in the Block-Centered-Flow input file not specified above are input according to standard MODFLOW requirements.

When the Strongly Implicit Procedure (SIP) file is selected, the preprocessor defaults parameters as follows:

- MXITER = 100, NPARM = 5
- ACCL = 1.0, HCLOSE = 100.0, IPCALC = 1, WSEED = blank IPRSIP = 100.

When the Slice-Successive Overrelaxation (SOR) file is selected, the preprocessor defaults parameters as follows:

- MXITER = 100
- ACCL = 1.0, HCLOSE = 100.0, IPRSOR = 100.

HCLOSE is large by hydraulic standards; however, recall that P^2 in cgs units is a large number ($\sim 10^{12}$).

The preprocessor creates an output file, MODEL.DAT, which contains the following information:

- selections for unit system
- number of wells and trenches
- elevation of ground surface, depth of atmospheric layer, temperature of the air being modeled
- depth to bottom of each modeled layer from ground
- extent of each well, including start and end cells in row, column, and layer directions and well pressure
- extent of each trench, including start and end cells in row, column, and layer directions and trench pressure.

MODEL.DAT must be present when the postprocessor is invoked.

3.1.6 PREAIR Unit System

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

- length units, where
  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

- volume units, where
  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

- time units, where
  1 s = 1.6667×10^{-2} min = 2.7778×10^{-4} hr = 1.1574×10^{-5} day = 3.1688×10^{-8} yr

- pressure units, where
  1 atm = 760 mmHg = 406.794 in. H_2O = 101.325 kPa = 14.696 lb/in^2

- temperature units, where
  °Celsius = °Kelvin - 273.15 = (°Fahrenheit - 32) / 1.8

- mass units, where
  1 g = 1.0 x 10-3 kg = 2.2046 x 10-3 lb

- permeability units, where
  1 cm2 = 1.0 x 10-2 dm2 = 1.0 x 10-4 m2 = 1.550 x 10-1 in2
  = 1.076 x 10-3 ft2 = 1.1962 x 10-4 yd2 = 1.0 x 108 darcy

The user can select any combination of the above unit systems, providing that all data are entered in the selected system. If no unit system is specified, PREAIR defaults to the first option for each item listed above.

3.1.7 PREAIR Constants

The following constants are defined in PREAIR:

- VAS = 0.000176 (viscosity of air at TVAS, in units of g/cm-s)
- TVAS = 283.15 (temperature at which VAS applies, in Kelvin)
- STDATM = 1013250.0 (1 atm = 1013250.0 g/cm-s2).

Note that the viscosity (μ) of an ideal gas is independent of pressure but dependent on the temperature (T) as follows:

$$\mu = \mu_R (T/T_R)^{1/2} \qquad (22)$$

where

μ_R = reference viscosity at T_R, and
T_R = reference temperature = TVAS.

The user can specify a value for the temperature of the air in the unsaturated zone. The preprocessor then calculates a corrected air-phase viscosity according to equation (22). If no air-temperature value is specified, the program uses the above reference values. In the preprocessor, the air viscosity is used only to calculate the pneumatic equivalent of the storage coefficient. This value is not required for steady-state simulations; however, the air viscosity is used in the postprocessor to correct both volumetric and mass-flow-rate output from MODFLOW. The specified or default value for the air temperature is transferred to the postprocessor through the MODEL.DAT file as described in Section 3.3.10.

The above settings should remain constant. If changes become necessary, the user must redefine values within PREAIR and then recompile the program so that the changes are incorporated in the executable program code.

3.2 PREAIR System Configuration

Load the source code PREAIR.FOR (on personal computers) or PREAIR.F77 (on mainframes) into an editing package on the computer system and check for compatibility with the operating environment.

3.2.1 Mainframe or Personal Computers

For operation on a mainframe computer, the following sections of code should appear in the main calling program:

```
C4----ASSIGN INPUT UNIT AND PRINTER UNIT
C
C    SET  :  IV(81) = INBAS = 5 WHEN USING IBM PC OR MAC
C    SET  :  IV(81) = INBAS = 1 WHEN USING MAIN FRAME
C    SET  :  IV(82) = IOUT  = 6 WHEN USING IBM PC OR MAC
C    SET  :  IV(82) = IOUT  = 1 WHEN USING MAIN FRAME
C
     INBAS = 1
     IOUT  = 1
C
C5---DEFINE UNIT NUMBER FOR BASIC PACKAGE
C
C    SET  :  LOCAT = 1 WHEN USING PERSONAL COMPUTER
C    SET  :  LOCAT = 5 WHEN USING MAIN FRAME OR MAC
     LOCAT = 5
```

For operation on a personal computer, the following sections of code should appear in the main calling program:

```
C4----ASSIGN INPUT UNIT AND PRINTER UNIT
C
C    SET  :  IV(81) = INBAS = 5 WHEN USING IBM PC OR MAC
C    SET  :  IV(81) = INBAS = 1 WHEN USING MAIN FRAME
C    SET  :  IV(82) = IOUT  = 6 WHEN USING IBM PC OR MAC
C    SET  :  IV(82) = IOUT  = 1 WHEN USING MAIN FRAME
C
     INBAS = 5
     IOUT  = 6
C
C5---DEFINE UNIT NUMBER FOR BASIC PACKAGE
C
C    SET  :  LOCAT = 1 WHEN USING PERSONAL COMPUTER
C    SET  :  LOCAT = 5 WHEN USING MAIN FRAME OR MAC
     LOCAT = 1
```

3.2.2 Array Dimensions

Memory allocation for the arrays in the air-flow preprocessor is specified by using two arrays, one real array XX(LENX) and one integer array IX(LENI). The size of the arrays is specified by a PARAMETER statement in the main program. For program applications on a mainframe or personal computer, the array size can be redefined to meet the system capacity. The preprocessor performs a check to determine whether the model storage requirements are adequate for the proposed application. If the allocated storage requirements are exceeded, the user must lengthen the arrays by increasing the values of LENX or LENI in the PARAMETER statement in the main code. The following section of code from the subroutine SETUP shows the storage-space check performed and the accompanying output message.

```
      IF (IV(28).GT.LENX) THEN
        WRITE(IOUT,250)
        WRITE(IOUT,251)IV(28)+1
        WRITE(IOUT,252)
        STOP
      END IF
 250 FORMAT(//////////////////////////////)
 251 FORMAT(T10,'REDIMENSION XX ARRAY TO LENX = ',I10)
 252 FORMAT(//,T10,'AND RECOMPILE PROGRAM')
      IMMX = IV(44)
      IF (IMMX.LT.IV(46)) IMMX = IV(46)
      IF (IMMX.GT.LENI) THEN
        WRITE(IOUT,261)
        WRITE(IOUT,262)IMMX+1
        WRITE(IOUT,263)
        STOP
      END IF
 261 FORMAT(//////////////////////////////)
 262 FORMAT(T10,'REDIMENSION IX ARRAY TO LENI = ',I10)
 263 FORMAT(//,T10,'AND RECOMPILE PROGRAM')
```

If either of the above messages appears during operation of the program, modify the following section of code from the main program according to the output recommendations:

```
C
C3---SPECIFICATIONS:
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      PARAMETER(LENX=500000,LENI=50000)
      COMMON XX(LENX),IX(LENI)
```

3.2.3 Compilation and Execution of PREAIR on a Mainframe or Personal Computer

Whenever modifications or changes are made to the program source code, the program must be recompiled so that the alterations are incorporated in the executable version of the program code. Because the program is written in Fortran 77, any standard Fortran 77 compiler can be used to recompile the code.

The following lines comprise a CPL file used on a PRIME mainframe computer to compile and run the air-flow preprocessor. Job-control language is specific to the compiler and the computer system. Adjustments to the commands below most likely will be necessary for your computing environment.

```
F77 PREAIR.F77
&DATA SEG -LOAD
LOAD PREAIR
LI
SA
QU
&END
SEG PREAIR
```

Commands needed to compile the air-flow preprocessor on a personal computer depend on the system and type of compiler being used. The following commands were used to compile and link the preprocessor on an IBM personal computer with Microsoft's Fortran compiler:

```
FL PREAIR.FOR
```

To run the preprocessor on a personal computer, make current the directory that contains the program executable code and, at the prompt, enter:

```
PREAIR
```

With both mainframe and personal computers, the introductory screen shown next will appear, prompting the user to select a particular option.

```
PREAIR - AN AIRFLOW PREPROCESSOR (Ver 1.1)
======  ==  ========  =============  ======

DEVELOPED BY :  ARTHUR L. BAEHR

                CRAIG J. JOSS

 SELECT :

1. TO RUN PREAIR WITH AN EXISTING INPUT FILE

2. TO MODIFY AN EXISTING INPUT FILE

3. TO CREATE A NEW DATA INPUT FILE

4. TO EXIT PREAIR


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

In order to use Option 1 and Option 2, the data files INFILEx.PRE (Section 3.3.3) and DATAIR.PRE (Section 3.3.4) must exist. Upon selecting 1 or 2, the user will be prompted for the name of the INFILEx.PRE file. For Option 1, the simulation will then create the MODFLOW input files. For Option 2, the contents of INFILEx.PRE will be displayed on the screen in sequence. The user can then change the data by entering a new value or can retain the existing data simply by pressing the ENTER or CARRIAGE RETURN key. After completing the changes, PREAIR saves the modified INFILEx.PRE file and returns the user to the above menu. The simulation can then proceed with the selection of Option 1.

Option 3 can be used to specify data in the file INFILEx.PRE. The current version (Ver 1.1) of PREAIR does not support the creation or modification of the file DATAIR.PRE. The file DATAIR.PRE must be created by the user. After creating INFILEx.PRE with Option 3, the program returns to the above menu, where the user can proceed with the simulation (Option 1), make additional changes to INFILEx.PRE (Option 2), or exit PREAIR (Option 4).

Option 4 is used to exit the program. After successful application of the preprocessor, a message is displayed that describes additional commands required to complete the AIR3D simulation. The display is shown next.

```
PREAIR - AN AIRFLOW PREPROCESSOR (Ver 1.1)
======   ==  ========  =============     ======

PREAIR has successfully set up the MODFLOW data files.

Next run MODFLOW, Enter :

MODFLOW < INFILE.MOD

When complete, run POSTAIR, Enter :

POSTAIR

Then use file INFILE.POS to input or modify POSTAIR data.
```

The command to run MODFLOW shown above allows input-file names to be entered directly into MODFLOW from the file INFILE.MOD. The procedure can be used with most personal computers. Other computing systems may require a different input format. At a minimum, the file INFILE.MOD can be used to obtain the input-file names required by MODFLOW. Depending on the model configuration and the computing system, run time can range from a few minutes to several hours. During the application of MODFLOW, text indicating unit numbers for input data files may be displayed on the computer screen. The successful application of MODFLOW will be indicated by the reappearance of the prompt on the computer screen.

The final step in implementing AIR3D is to run the postprocessor, POSTAIR. The above commands for running POSTAIR apply only to personal computers. The input file INFILEx.POS (Section 4.5.3) required by POSTAIR is created with the preprocessor by assigning default values to input variables. Depending on the model application, INFILEx.POS can be used directly with POSTAIR or modified by using POSTAIR to select specific output options. Output-file names are specified within the postprocessor (see Section 4.4). The user can then access the binary or ASCII text output files with commercially available editing, graphical, spreadsheet, or statistical software.

3.3 PREAIR Input/Output Files

3.3.1 PREAIR Input Files

Two input files are required to run PREAIR:

- INFILEx.PRE (Section 3.3.3)
- DATAIRx.PRE (Section 3.3.4).

INFILEx.PRE is specified interactively by the user after invoking PREAIR. INFILEx.PRE contains the name of the other preprocessor input file (for example, DATAIRx.PRE); the names of the output files created by the preprocessor, which serve as input to MODFLOW (for example, BASAIRx.PRN, OCAIRx.PRN...); the names of MODFLOW output files (for example, HEADx.BIN, FLOWx.BIN); and the input-file name for the postprocessor (for example, INFILEx.POS). Note that the data in INFILEx.PRE can be specified by using Option 2 in the preprocessor main menu (Run PREAIR Interactively).

DATAIRx.PRE is read directly by PREAIR. DATAIRx.PRE contains the geometric, geologic, and pneumatic information required for the model. Note that the file DATAIRx.PRE must be created before the preprocessor is run.

3.3.2 PREAIR Output Files

The purpose of the preprocessor PREAIR is to interpret input that defines an air-flow simulation so that the finite-difference approximation to the air-flow equation can be solved with MODFLOW. MODFLOW input files are created by the preprocessor (PREAIR output files). Four files are required as input to MODFLOW and are named in the input file INFILEx.PRE, as follows:

- BASAIRx.PRN (Section 3.3.5)
- OCAIRx.PRN (Section 3.3.6)
- BCFAIRx.PRN (Section 3.3.7)
- SIPAIRx.PRN or SORAIRX.PRN (Section 3.3.8).

The data format for the previous input files is the same as that defined in the documentation of MODFLOW. Many variables in the input files are defaulted to standard values for air-flow simulations by the preprocessor to reduce data-input requirements. Binary output files for saving head and cell-by-cell flow values are specified automatically by the preprocessor. Similarly, information written to the MODFLOW text output files is minimized by using default values. Note also that the following MODFLOW packages do not apply to air-flow simulations:

- River Package
- Recharge Package
- Well Package
- Drain Package
- Evapotranspiration Package
- General Head Boundary Package.

MODFLOW input- and output-file names specified in the file INFILEx.PRE are organized by PREAIR and written to a file for subsequent use with MODFLOW. The file is called INFILE.MOD (Section 3.3.9).

Depending on the computer system used, INFILE.MOD can be used either directly with MODFLOW (Section 3.2.3) or as a list to assist the user in implementing MODFLOW. In either case, INFILE.MOD provides a record of the MODFLOW input-file names as well as the names of the MODFLOW binary output files.

A sixth file is created by PREAIR for direct use in the postprocessor (not required by MODFLOW). This file is called MODELx.DAT (Section 3.3.10). This file is used to transfer selected information, such as physical unit system, well/trench information, physical properties, and layer depths, from the preprocessor to the postprocessor. Note that the name of the file, MODELx.DAT, is specified within the pre- and postprocessor input files (INFILEx.PRE and INFILEx.POS), and that consistency in naming the file is required.

The final file generated by PREAIR is the input file for the postprocessor. This file is named INFILEx.POS (Section 3.3.11) in the input file INFILEx.PRE. INFILEx.POS records file names required by the postprocessor as well as default output values. After POSTAIR is invoked, a menu appears that allows the user to choose either to complete the air-flow simulation by using the created INFILEx.PRE file directly, to modify the file, or to set up a new INFILEx.POS file before proceeding with the simulation.

Format statements used in the data input and output follow Fortran 77 conventions, namely Ixx for integers, Fxx.xx for real numbers, Exx.xx for exponential numbers, and Axx for character input. Note that in reading data with a format of F10.0 the user can insert the location of the decimal point.

3.3.3 PREAIR Input File INFILEx.PRE

INFILEx.PRE file specifications are as follows:

Name of file:	Specified by the user after invoking the preprocessor (for example, INFILEx.PRE)
File contents:	Name of file with preprocessor input data, name of output file containing data for Basic Package, name of output file containing data for Output-Control Package, name of output file containing data for Block-Centered-Flow Package, name of output file containing data for Matrix-Solver (SIP or SOR) Package, name of file containing binary head output, name of file containing binary flow output, name of data-transfer file, name of postprocessor input file.

File application:	This file is used to specify names of input and output files associated with the air-flow preprocessor PREAIR.
Fortran unit number:	The program defines the INFILEx.PRE input file as UNIT=11.
Program input:	Input from INFILEx.PRE is read in the subroutine SETUP.

INFILEx.PRE contains the names of files used to store data for the simulation. INFILEx.PRE consists of nine lines of input, each containing a file name in A12 format as follows:

```
                                               Input records
Data    Fortran Name                          |---|---|---|
item    (A12 Format)                          1   5   10  15

 1.     FNAME(2)------------------------------DATAIR4.PRE
 2.     FNAME(3)------------------------------BASAIR4.PRN
 3.     FNAME(4)------------------------------OCAIR4.PRN
 4.     FNAME(5)------------------------------BCFAIR4.PRN
 5.     FNAME(6)------------------------------SIPAIR4.PRN
 6.     FNAME(7)------------------------------HEAD4.BIN
 7.     FNAME(8)------------------------------FLOW4.BIN
 8.     FNAME(9)------------------------------MODEL4.DAT
 9.     FNAME(11)-----------------------------INFILE4.POS
```

where
FNAME(2) is the name of the file used to input air-flow-model information into the air-flow preprocessor PREAIR. FNAME(2) must be specified in order to implement the air-flow preprocessor.

FNAME(3) is the name of the file used to create data needed for the Basic Package in MODFLOW. FNAME(3) defaults to the name BASAIR.PRN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(4) is the name of the file used to create data needed for the Output Control Package in MODFLOW. FNAME(4) defaults to the name OCAIR.PRN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(5) is the name of the file used to create data needed for the Block-Centered-Flow Package in MODFLOW. FNAME(5) defaults to the name BCFAIR.PRN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(6) is the name of the file used to create data needed for the selected matrix-solver procedure, either the Strongly Implicit Procedure (SIP) or the Slice Successive Overrelaxation Procedure (SOR), in MODFLOW. FNAME(6) defaults to the setting SIPAIR.PRN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(7) is the name of the file that contains binary head output from MODFLOW. FNAME(7) defaults to the name HEAD.BIN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(8) is the name of the file that contains binary flow output from MODFLOW. FNAME(8) defaults to the name FLOW.BIN if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(9) is the name of the file used to transfer selected model information between the pre- and postprocessors. The file name FNAME(9) is entered interactively into the postprocessor by the user. FNAME(9) defaults to the name MODEL.DAT if no name is specified by the user. Note that a blank line must be entered if no name is specified.

FNAME(11) is the name of the file used to output information and file names from PREAIR for subsequent use in POSTAIR. The file name FNAME(11) is entered interactively when using the postprocessor. FNAME(11) defaults to the name INFILEx.POS if no name is specified by the user. Note that a blank line must be entered if no name is given.

The name INFILEx.MOD is assigned by the preprocessor to location FNAME(10). INFILE.MOD records MODFLOW input-file names. The name MODAIR.PRN is assigned by the preprocessor to FNAME(12). MODAIR.PRN is the name of the file used by MODFLOW to output text information pertaining to the simulation. The contents of MODAIR.PRN are not transformed into dimensionally consistent pneumatic parameters; therefore, the information in this file is not directly useful.

3.3.4 PREAIR Input File DATAIRx.PRE

DATAIRx.PRE file specifications are as follows:

Name of file:	Specified by user in file INFILEx.PRE (for example, DATAIRx.PRE)
File contents:	Simulation heading; physical unit system; number of model layers, rows, and columns; number of stress periods, wells, and trenches; SIP or SOR selection; atmospheric pressure; well and trench locations; simulation duration; number of time steps; time step-multiplier; transient or steady state indicator; grid dimensions in row and column directions; ground-surface elevation; air temperature; atmospheric parameters; layer characterization and other geologic parameters.

File application:	This file is used to input discretization, pneumatic, and geologic data into the preprocessor.
Fortran unit number:	The program defines the DATAIRx.PRE input file as UNIT=12.
Program input:	Input from DATAIRx.PRE is performed in the following subroutines: STOR, MODBAS, and MODBCF.
Parameter 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 parameter.

The structure of DATAIRx.PRE and format of data input are given below. Fortran variables are defined at the end of this section.

1. Data: HEAD1
   Format: 20A4

2. Data: HEAD2
   Format: 12A4

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

4. Data: NLAY,NROW,NCOL,NPER
   Format: 4I10

5. Data: LTYPE,NWELL,NTRCH
   Format: 3I10

6. Data: NSOLV
   Format: I10

7. Data: ATM
   Format: F10.0

Input item 8 is not needed if no wells are present (NWELL=0). One record is needed for each of the NWELLs specified. Note that IW=1,2,...,NWELL.

8. Data: IWELL(IW,1),IWELL(IW,2),IWELL(IW,3),IWELL(IW,4),IWELL(IW,5), IWELL(IW,6), IWELL(IW,7),SHW(IW)
   Format: 7I5,F10.0

Input item 9 is not needed if no trenches are present (NTRCH=0). One record is needed for each of the NTRCH trenches specified. Note that IT=1,2,...,NTRCH.

9. Data: ITRCH(IT,1),ITRCH(IT,2),ITRCH(IT,3),ITRCH(IT,4),ITRCH(IT,5), ITRCH(IT,6),ITRCH(IT,7),TSHD(IT)
   Format: 7I5,F10.0

Input item 10 requires a record for each of NPER stress periods.

10. Data: PERLEN,NSTP,TSMULT
    Format: F10.0,I10,F10.0

11. Data: ISS
    Format: I10

12. Data: CDIST,IVV1,FMTIN
    Format: F10.0,I10,5A4

Input item 13 is not needed if cell spacing is uniform in the column direction (IVV1=0). If IVV1=1 (that is nonuniform cell spacing in column direction) then item 13 requires NROW records. Note that IC=1,2,..,NROW.

13. Data: DELC(IC)
    Format: FMTIN

14. Data: RDIST,IVV2,FMTIN
    Format: F10.0,I10,5A4

Input item 15 is not needed if cell spacing is uniform in the row direction (IVV2=0). If IVV2=1 (that is nonuniform cell spacing in row direction) then item 15 requires NCOL records. Note that IR=1,2,..,NCOL.

15. Data: DELR(IR)
    Format: FMTIN

16. Data: GELEV,TAIR,BSURF,XVKSRF
    Format: 3F10.0,E10.3

Program input after this point will depend on value of LTYPE:

If the properties within a layer are constant, then LTYPE=1 and items 17 and 18 are defined as follows. If properties within a layer vary, omit items 17 and 18.

17. Data: NGEOL,DTOT
    Format: I10,F10.0

Input Item 18 NGEOL times (one record each layer).

18. Data: NGL,INMLB,XDEEP,XKX,YKRAT,XKZ,AIRP
    Format: I10,I10,F10.0,E10.3,F5.0,E10.3,F5.0

If the properties within any layer are not uniform, then LTYPE=2 and items 19 through 27 are defined as follows. Omit items 19 through 27 if LTYPE=1.

Item 19 is the anisotropy ratio, k_y/k_x, for the layer. For isotropic conditions, set LOCAT=0 and CNSTNT=1.0, and leave FMTIN blank.

19. Data: LOCAT,CNSTNT,FMTIN
    Format: I10,F20.0,5A4

If LOCAT>0 (anisotropy) then item 20 requires a record for each of NLAY layers. Note that IP=1,2,...NLAY. Omit item 20 if LOCAT=0 (isotropic conditions).

20. Data: TRPY(IP)
    Format: FMTIN

A subset of data items 21 through 27 is used to describe each layer. With the exception of the array defining the air-phase porosity, all other parameters must be entered. The air-phase-porosity array is entered only if the simulation is transient (ISS=0); the air-phase porosities are used to calculate the pneumatic equivalent of storage coefficient. If the simulation is steady-state (ISS≠0), the air-phase-porosity arrays are omitted. Data items 21 through 27 are read in as a block for each layer; that is, items 21 through 27 for layer 1 are read first, then items 21 through 27 for layer 2, and so on, as is done in MODFLOW. If input parameters are constant within a layer, either use the abbreviated form (LOCAT = 0) and omit the array input, or define the values at each cell in the two-dimensional text arrays (for LOCAT > 0) or the two-dimensional binary arrays (for LOCAT < 0). See the Utility Input documentation for U2DREL in the MODFLOW manual for further explanations of this mode of data input.

Input items 21 through 27 as a block NLAY times (once for each layer).
Input item 21 (cell depth in layer or Z-direction). The program accepts only constant-cell depths; therefore, LOCAT=0, CNSTNT=layer depth, and FMTIN is left blank.

21. Data: LOCAT,CNSTNT,FMTIN
    Format: I10,F20.0,5A4

Input item 22 (air-phase permeability in layer or Z-direction).

22. Data: LOCAT,CNSTNT,FMTIN,IFLAG2
    Format: I10,F20.0,5A4,I10

If LOCAT>0 (nonuniform vertical permeability, text input option) then input item 23 as a two-dimensional text array (IR=1,...,NROW) for each layer. Omit item 23 if LOCAT=0.

23a. Data: VPERM2(1,IR),VPERM2(2,IR),....,VPERM2(NCOL,IR)
     Format: FMTIN

If LOCAT<0 (nonuniform vertical permeability, binary input option) then input item 23 as binary data (IR=1,...,NROW). Omit item 23 if LOCAT=0.

23b. Data: VPERM2(1,IR),VPERM2(2,IR),....,VPERM2(NCOL,IR)
     Format: binary

If ISS=0 (transient simulation) then input items 24 and 25 (air-phase porosity). Omit item 24 if ISS≠0.

24. Data: LOCAT,CNSTNT,FMTIN
    Format: I10,F20.0,5A4

If LOCAT>0 (nonuniform air-phase porosity, text input option) then input item 25 as a two-dimensional text array (IR=1,.,NROW). Omit item 25 if LOCAT=0.

25a. Data: VCONT(1,IR),VCONT(2,IR),.....,VCONT(NCOL,IR)
     Format: FMTIN

If LOCAT<0 (nonuniform air-phase porosity, binary input option) then input item 25 as binary data (IR=1,...,NROW). Omit item 25 if LOCAT=0.

25b. Data: VCONT(1,IR),VCONT(2,IR),.....,VCONT(NCOL,IR)
     Format: binary

Input item 26 (horizontal air-phase permeability along rows).

26. Data: LOCAT,CNSTNT,FMTIN
    Format: I10,F20.0,5A4

If LOCAT>0 (nonuniform horizontal permeability, text input option) then input item 27 as a two-dimensional text array (IR=1,.,NROW). Omit item 27 if LOCAT=0.

27a. Data: XPERM(1,IR),XPERM(2,IR),.....,XPERM(NCOL,IR)
Format: FMTIN

If LOCAT<0 (nonuniform horizontal permeability) then input item 27 as binary data (IR=1,,NROW). Omit item 27 if LOCAT=0.

27b. Data: XPERM(1,IR),XPERM(2,IR),.....,XPERM(NCOL,IR)
Format: binary

An example of DATAIRx.PRE for LTYPE = 1 is given below:

Data item	Explanation	Input records (columns 1 5 10 15 20 25 30 35 40 45 50 55 60)
1.	HEAD1	3 DIMENSIONAL AIR FLOW ANALYSIS (UNIFORM LAYER PROPERTIES)
2.	HEAD2	3 LAYS, 5 ROWS, 7 COLS
3.	IU1(1),IU1(2),.....,IU1(6),IU1(7)	1 1 1 1 1 1 1
4.	NLAY,NROW,NCOL,NPER	3 5 7 1
5.	LTYPE,NWELL,NTRCH	1 1 0
6.	NSOLV	1
7.	ATM	1.00
8.	IWELL(I,1),........,IWELL(I,7),SHW(I)	1 3 3 4 4 2 2 0.900
10.	PERLEN,NSTP,TSMULT	3600.00 1 1.0
11.	ISS	1
12.	CDIST,IVV1,FMTIN	500.0 0
14.	RDIST,IVV2,FMTIN	700.0 0
16.	GELEV,TAIR,BSURF,XVKSRF	
17.	NGEOL,DTOT	2 300.0
18a.	NGL,INMLB,XDEEP,XKX,YKRAT,XKZ,AIRP	1 1 100.0 1.000E-08 1.0 1.000E-09 0.30
18b.	NGL,INMLB,XDEEP,XKX,YKRAT,XKZ,AIRP	2 3 200.0 2.000E-08 1.0 2.000E-09 0.25

An example of DATAIRx.PRE for LTYPE = 2 is given below:

```
                                                      Input records
Data                Explanation                ├──┼────┼────┼────┼────┼────┼────┼────┼────┼────┼────┼────┤
item                                           1  5    10   15   20   25   30   35   40   45   50   55   60

 1.  HEAD1────────────────────────────────────3 DIMENSIONAL AIR FLOW ANALYSIS (NON-UNIFORM LAYER PROPERTIES)
 2.  HEAD2──────────────────────────────────── 3 LAYS, 5 ROWS, 7 COLS
 3.  IU1(1),IU1(2),....,IU1(6),IU1(7)────────     1    1    1    1    1    1    1
 4.  NLAY,NROW,NCOL,NPER──────────────────────         3         5         7         1
 5.  LTYPE,NWELL,NTRCH────────────────────────         2         1         0
 6.  NSOLV────────────────────────────────────         1
 7.  ATM──────────────────────────────────────      1.00
 8.  IWELL(I,1),.......,IWELL(I,7),SHW(I)─────    1    3    3    4    4    2    2    0.900
10.  PERLEN,NSTP,TSMULT───────────────────────   3600.00         1       1.0
11.  ISS──────────────────────────────────────         1
12.  CDIST,IVV1,FMTIN─────────────────────────     500.0         1(5F10.1)
13.  DELC(1),DELC(2),DELC(3),DELC(4),DELC(5)-     100.0     100.0     100.0     100.0     100.0
14.  RDIST,IVV2,FMTIN─────────────────────────     700.0         1(6F10.1)
15.  DELR(1),.......DELR(6)───────────────────     100.0     100.0     100.0     100.0     100.0     100.0
15.  DELR(7)──────────────────────────────────     100.0
16.  GELEV,TAIR,BSURF,XVKSRF──────────────────       0.0      10.0      20.0 1.000E-07
19.  LOCAT,CNSTNT,FMTIN───────────────────────         0                 1.0
21.  LOCAT,CNSTNT,FMTIN──────────(layer 1)────         0               100.0
22.  LOCAT,CNSTNT,FMTIN,IFLAG2───(layer 1)────        12         0.000000001(6F10.3)
23a. VPERM2(1,1),VPERM2(2,1),..,VPERM2(6,1)──     1.000     1.000     1.000     1.000     1.000     1.000
23a. VPERM2(7,1)──────────────────────────────     1.000
23a. VPERM2(1,2),VPERM2(2,2),..,VPERM2(6,2)──     1.000     1.000     1.000     1.000     1.000     1.000
23a. VPERM2(7,2)──────────────────────────────     1.000
23a. VPERM2(1,3),VPERM2(2,3),..,VPERM2(6,3)──     1.000     1.000     1.000     1.000     1.000     1.000
23a. VPERM2(7,3)──────────────────────────────     1.000
23a. VPERM2(1,4),VPERM2(2,4),..,VPERM2(6,4)──     1.000     1.000     1.000     1.000     1.000     1.000
23a. VPERM2(7,4)──────────────────────────────     1.000
23a. VPERM2(1,5),VPERM2(2,5),..,VPERM2(6,5)──     1.000     1.000     1.000     1.000     1.000     1.000
23a. VPERM2(7,5)──────────────────────────────     1.000
```

Data Item	Explanation (Continued)	1 5 10	15 20	25 30	35 40	45 50	55 60
26a.	LOCAT,CNSTNT,FMTIN————(layer 1)—	12	0.00000001(6F10.3)				
27a.	XPERM(1,1),XPERM(2,1),..,XPERM(6,1)——	1.000	1.000	1.000	1.000	1.000	1.000
27a.	XPERM(7,1)——————————	1.000					
27a.	XPERM(1,2),XPERM(2,2),..,XPERM(6,2)——	1.000	1.000	1.000	1.000	1.000	1.000
27a.	XPERM(7,2)——————————	1.000					
27a.	XPERM(1,3),XPERM(2,3),..,XPERM(6,3)——	1.000	1.000	1.000	1.000	1.000	1.000
27a.	XPERM(7,3)——————————	1.000					
27a.	XPERM(1,4),XPERM(2,4),..,XPERM(6,4)——	1.000	1.000	1.000	1.000	1.000	1.000
27a.	XPERM(7,4)——————————	1.000					
27a.	XPERM(1,5),XPERM(2,5),..,XPERM(6,5)——	1.000	1.000	1.000	1.000	1.000	1.000
27a.	XPERM(7,5)——————————	1.000					
21.	LOCAT,CNSTNT,FMTIN————(layer 2)—	0		100.000			
22.	LOCAT,CNSTNT,FMTIN,IFLAG2—(layer 2)—	0		0.000000002			
26.	LOCAT,CNSTNT,FMTIN————(layer 2)—	0		0.00000002			
21.	LOCAT,CNSTNT,FMTIN————(layer 3)—	0		100.000			
22.	LOCAT,CNSTNT,FMTIN,IFLAG2—(layer 3)—	0		0.000000002			
26.	LOCAT,CNSTNT,FMTIN————(layer 3)—	0		0.00000002			

The definition of Fortran variables required in the DATAIRx.PRE file is presented below. Variables are presented in the order in which they appear in the data file. The user can select the most convenient unit systems for the input and output of data. If no unit systems are specified, input must conform to the system defined in section 3.1.6.

HEAD1

- HEAD1 is a simulation heading or description identifying the simulation. The definition is the same as that for HEADING in the MODFLOW documentation.
- HEAD1 is for descriptive purposes only and is not needed to implement the air-flow preprocessor. If HEAD1 is not used, a blank line must be inserted in the data file.
- Input length must not exceed 80 characters (20A4).

HEAD2

- HEAD2 is a simulation heading or description identifying the simulation. The definition is the same as that for HEADING in the MODFLOW documentation.
- HEAD2 is for descriptive purposes only and is not needed to implement the air-flow preprocessor. If HEAD2 is not used, a blank line must be inserted in the data file.
- Input length must not exceed 48 characters (12A4).

IU1(1)

- IU1(1) is the specification for input and output 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).
- 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.
- The input format is I5.

IU1(2)

- IU1(2) is the specification for input and output 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).

  The unit system selected applies to all volume units in the input and output data files. Note that the volumetric unit system does not need to correspond with 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.
- The input format is I5.

IU1(3)

- IU1(3) is the specification for input and output 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).

  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, per minute, per hour, per day, or per year, respectively.
- IU1(3) defaults to a value of 1 (time units in seconds) when no value is specified by the user.
- The input format is I5.

IU1(4)

- IU1(4) is the specification for input and output 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 of Hg),
  IU1(4) = 3 for pressure in units of inches of water (in. of 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).
  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.
- The input format is I5.

IU1(5)

- IU1(5) is the specification for input and output 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).
  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.
- The input format is I5.

IU1(6)

- IU1(6) is the specification for input and output 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).
  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 unit time, kg per unit time, and lb per unit time.
- IU1(6) defaults to a value of 1 (mass units in grams) when no value is specified by the user.
- The input format is I5.

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.

  The unit system selected applies to all permeability values 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.
- The input format is I5.

NLAY
- NLAY is the number of cell layers in the model. Note that the program superimposes an additional layer (layer 0) on the model to represent atmospheric conditions. The definition of NLAY is the same as that in the MODFLOW documentation.
- The input format is I10.

NROW
- NROW is the number of model rows specified by the user. The definition of NROW is the same as that in the MODFLOW documentation.
- The input format is I10.

NCOL
- NCOL is the number of model columns specified by the user. The definition of NCOL is the same as that in the MODFLOW documentation.
- The input format is I10.

NPER
- NPER is the number of stress periods in the simulation. The definition of NPER is the same as that in the MODFLOW documentation.
- The input format is I10.

LTYPE
- LTYPE serves as a flag to indicate the nature of the geologic input to follow. LTYPE = 1 for uniform properties within geologic units that consist of one or more cell layers (that is, parameters within a geologic unit are the same at every cell location). LTYPE = 2 is used to model general variable properties within the model cell layers (that is, parameters within each cell layer can vary in the row and column directions). The value specified for LTYPE determines the format of input data from the file DATAIRx.PRE as indicated below. LTYPE does not appear in the MODFLOW documentation.
- The input format is I10.

NWELL
- NWELL is the number of wells specified by the user. Note that one well can encompass several model cells; hence, starting and ending rows, columns, and layers are required for each well. Note that, in air-flow simulations, well cells are assigned constant pressure with the pressure equal to the applied well vacuum or pressure squared (see Section 3.1.3). Wells differ from trenches in that the model cells above a well are designated as no-flow cells to emulate the well riser pipe. Pressure output at no-flow cells appears as a value of 1000 when the units are atmospheres.
- A value of NWELL=0 is acceptable to simulate natural air-flow corresponding to atmospheric-pressure variation.
- The input format is I10.

NTRCH

- NTRCH is the number of trenches specified by the user. Note that one trench can encompass several model cells; hence, starting and ending rows, columns, and layers are required for each trench. Trench cells are constant-pressure cells (see Section 3.1.3). NTRCH does not appear in the MODFLOW documentation. Trenches differ from wells in that the model cells above a trench are designated as flow cells.
- A value of NTRCH=0 is acceptable.
- The input format is I10.

NSOLV

- NSOLV is the flag that specifies the matrix-solver package in MODFLOW. To specify the SIP package, set NSOLV=1. To specify the SOR package, set NSOLV=2. Depending on the value selected, the preprocessor assigns a unit number to the SIP (unit 8) or SOR (unit 9) package.
- NSOLV defaults to a value of 1 (SIP option) if no (or an incorrect) value is specified by the user.
- The input format is I5.

ATM

- ATM is the prevailing atmospheric pressure for the simulation. The preprocessor converts the input from the specified pressure unit system to units of centimeters-grams-seconds and then uses ATM^2 for the initial conditions in the model domain.
- ATM must be specified in order to implement the air-flow preprocessor.
- Only a real value is accepted.
- The physical units depend on IU1(4); the default is atmospheres.
- The input format is F10.0.

IWELL(IW,1)

- IWELL(IW,1) is an identification number assigned to each well.
- IWELL(IW,1) must be specified NWELL times.
- IWELL(IW,1) defaults to 1,2,3..and so on, if no value is specified.
- The input format is I5.

IWELL(IW,2)

- IWELL(IW,2) is the beginning row number for the range of cells encompassed by well number IWELL(IW,1).
- IWELL(IW,2) must be specified NWELL times.
- The input format is I5.

IWELL(IW,3)

- IWELL(IW,3) is the ending row number for the range of cells encompassed by well number IWELL(IW,1).
- IWELL(IW,3) must be specified NWELL times.
- The input format is (I5).

IWELL(IW,4)

- IWELL(IW,4) is the beginning column number for the range of cells encompassed by well number IWELL(IW,1).
- IWELL(IW,4) must be specified NWELL times.
- The input format is (I5).

IWELL(IW,5)

- IWELL(IW,5) is the ending column number for the range of cells encompassed by well number IWELL(IW,1).
- IWELL(IW,5) must be specified NWELL times.
- The input format is I5.

IWELL(IW,6)

- IWELL(IW,6) is the beginning layer number for the range of cells encompassed by well number IWELL(IW,1).
- IWELL(IW,6) must be specified NWELL times.
- The input format is I5.

IWELL(IW,7)

- IWELL(IW,7) is the ending layer number for the range of cells encompassed by well number IWELL(IW,7).
- IWELL(IW,7) must be specified NWELL times.
- The input format is I5.

SHW(IW)

- SHW(IW) is the pressure assigned to the cells of well number IWELL(IW,1).
- SHW(IW) is specified for each well.
- The physical units depend on IU1(4); the default is atmospheres.
- The input format is F10.0.

ITRCH(IT,1)

- ITRCH(IT,1) is an identification number assigned to each trench.
- ITRCH(IT,1) is specified NTRCH times.
- ITRCH(IT,1) defaults to 1,2,3..., and so on, if no value is specified.
- The input format is I5.

ITRCH(IT,2)

- ITRCH(IT,2) is the beginning row number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,2) is specified for each trench.
- The input format is I5.

ITRCH(IT,3)

- ITRCH(IT,3) is the ending row number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,3) is specified for each trench.
- The input format is I5.

ITRCH(IT,4)

- ITRCH(IT,4) is the beginning column number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,4) is specified for each trench.
- The input format is I5.

ITRCH(IT,5)

- ITRCH(IT,5) is the ending column number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,5) is specified for each trench.
- The input format is I5.

ITRCH(IT,6)

- ITRCH(IT,6) is the beginning layer number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,6) is specified for each trench.
- The input format is I5.

ITRCH(IT,7)

- ITRCH(IT,7) is the ending layer number for the range of cells encompassed by trench number ITRCH(IT,1).
- ITRCH(IT,7) is specified for each trench.
- The input format is I5.

TSHD(IT)

- TSHD(IT) is the specified pressure for the range of cells encompassed by trench number ITRCH(IT,1).
- TSHD(IT) is specified for each trench.
- The input format is F10.0.

PERLEN

- PERLEN is the length of the stress periods. PERLEN must be specified once for each stress period.
- The physical units depend on IU1(3); the default is seconds.
- The input format is F10.0.

NSTP

- NSTP is the number of time steps in a stress period. NSTP must be specified once for each stress period.
- The input format is I10.

TSMULT

- TSMULT is the multiplier for the length of successive time steps. TSMULT must be specified once for each stress period.
- The input format is F10.0.

ISS

- ISS specifies whether the simulation is steady-state (ISS=1) or transient (ISS=0). Note that, in many cases, air flow in the unsaturated domain rapidly approaches steady state. Therefore, in many cases analysis can be simplified to a steady-state problem.
- The input format is I10.

CDIST

- CDIST is the length of the domain in the column direction (Y-direction). If cells are of equal width along the columns, CDIST equals NROW multiplied by the row width.
- The physical units depends on IU1(1); the default is centimeters.
- The input format is F10.0.

IVV1

- IVV1 records whether cell widths along the model columns (in the Y-direction) are constant (IVV1=0) or variable (IVV1=1).
- If IVV1 = 0, then the program determines cell widths simply by dividing CDIST by NROW, and DELC(I) input is omitted.
- If IVV1 = 1, then the user must specify cell widths DELC(I).
- IVV1 defaults to 0 if no (or an incorrect) value is specified.
- The input format is I10.

FMTIN

- FMTIN is input only if IVV1 = 1 or IVV2 = 1.
- FMTIN is the format of records containing array values. It is used only if IVV1 > 0 or IVV2 > 0. The format must be enclosed in parentheses; for example: (6F10.3).
- The input format is 5A4.

DELC(I)

- DELC(I) is input only if IVV1 = 1.
- DELC(I) are the nonuniform cell widths in the column direction (in Y-direction).
- NROW values are required.
- The physical units depend on IU1(1); the default is centimeters.
- The input format is defined by FMTIN.

RDIST

- RDIST is the length of the domain in the row direction (in the X-direction). If cells are of equal width along rows, RDIST equals NCOL multiplied by column width.
- The physical units depend on IU1(1); the default is centimeters.
- The input format is F10.0.

IVV2

- IVV2 records whether cell widths along the model rows (in the X-direction) are constant (VV2=0) or variable (IVV2=1).
- If IVV2 = 0, the program determines cell widths simply by dividing RDIST by NCOL, and DELR(I) input is omitted.
- If IVV2 = 1, then the user must specify cell widths DELR(I).
- The input format is I10.

DELR(I)

- DELR(I) is input only if IVV2=1.
- DELR(I) are the nonuniform cell widths in the row direction (in the X-direction).
- NCOL values are required.
- The physical units depend on IU1(1); the default is centimeters.
- The input format depends on FMTIN.

GELEV

- GELEV is a reference value used to define the ground-surface elevation (the datum at the top of the uppermost layer specified by the user).
- Note that GELEV coincides with the bottom of the atmospheric layer superimposed on the model by the program.
- The program calculates elevations at the bottom of each cell layer relative to GELEV. For example, if GELEV = 0.0 cm and the model layers are 100.0 cm thick, the elevations at the bottoms of the layers will be -100.0 cm, -200.0 cm, and so on. Alternatively, for GELEV = 1,000.0 cm, the elevations at the bottoms of the layers will be +900.0 cm, +800 cm, and so on. GELEV, then, affects the values of the spatial Z-coordinate, which define the vertical locations of air-flow pressures and flow rates in the model domain.
- GELEV defaults to a value of 0.0 if no value is specified by the user.
- The physical units depend on IU1(1); the default is centimeters.
- The input format is F10.0.

TAIR

- TAIR is the average temperature of the domain.
- TAIR is used to correct the air viscosity, μ, which is specified by the preprocessor as μ_0=1.73 x 10^{-4} g/cm-s at 283.15 K, according to the following equation: $\mu=\mu_0((TAIR)/283.15)^{1/2}$.
- TAIR defaults to a value of 10°C if no value is specified.
- The physical units depend on IU1(5); the default is Celsius.
- The input format is F10.0.

BSURF

- BSURF is the depth of the additional cell layer superimposed on the model domain to ensure that the ground-surface boundary condition is specified as constant atmospheric pressure.
- BSURF and XVKSRF are used by the preprocessor to determine the vertical conductance of the superimposed atmospheric layer.
- When not specified by the user, BSURF defaults to a value of 0.2 times the thickness of the uppermost geologic cell layer in the model if this layer thickness is greater than or equal to 5.0 cm. BSURF defaults to 1.0 times the thickness of the uppermost geologic cell layer if this layer thickness is less than 5.0 cm. Use of default value together with the default value for XVSURF minimizes the effect of flow through the top layer.
- The physical units depend on IU1(1); the default is centimeters.
- The input format is F10.0.

XVKSRF

- XVKSRF is the vertical air-phase permeability of the additional cell layer superimposed on the model domain.
- BSURF and XVKSRF are used by the preprocessor to determine the vertical conductance of the superimposed atmospheric layer.
- When XVKSRF is not specified by the user, XVKSRF defaults to a value of 100 times the maximum value of the vertical permeability of the uppermost geologic cell layer. Use of this default value together with the default value for BSURF minimizes the effect of flow through the uppermost layer.
- The physical units depend on IU1(7); the default is centimeters squared.
- The input format is E10.3.

NGEOL

- NGEOL is input only if LTYPE = 1.
- NGEOL is the number of geologic units.
- A geologic unit can encompass several cell layers in the model. In such cases, the preprocessor assigns the specified geologic parameters to each of the cell layers that fall within the geologic unit.
- In cases where geologic properties vary throughout the domain (LTYPE=2), the user must define arrays with parameter values at each cell location.
- The input format is I10.

DTOT

- DTOT is input only if LTYPE = 1.
- DTOT is the depth of the model domain in the Z-direction (the sum of layer thicknesses).
- This value must equal the sum of the geologic unit thicknesses (XDEEP); if not, the program will end.
- The physical units depend on IU1(1); default is centimeters.
- The input format is F10.0.

NGL

- NGL is input only if LTYPE = 1.
- The geologic units are numbered, NGL=1 for the uppermost geologic unit, and NGL=NGEOL for the bottommost geologic unit.
- The input format is I10.

INMLB

- INMLB is input only if LTYPE = 1.
- Each geologic unit can contain multiple cell layers. INMLB is the layer number corresponding to the layer forming the bottom of each geologic unit. Note that INMLB is less than or equal to NLAY.
- The program performs a check to ensure the layer numbering is consistent with domain dimensions; if an error is found, the program ends.
- The input format is I10.

XDEEP

- XDEEP is input only if LTYPE = 1.
- XDEEP is the thickness of each geologic unit. A geologic unit can consist of several cell layers; the sum of the thicknesses of these layers equals XDEEP.
- The physical units depend on IU1(1); the default is centimeters.
- The input format is F10.0.

XKX

- XKX is input only if LTYPE = 1.
- XKX is the air-phase permeability of a geologic unit in the row direction (in the X-direction). The preprocessor multiplies XKX by cell depth to obtain a transmissivity, which is assigned to all cells within the geologic unit.
- The physical units depend on IU1(7); the default is centimeters squared.
- The input format is E10.3.

YKRAT

- YKRAT is input only if LTYPE = 1.
- YKRAT is the ratio of air-phase permeability in the column direction (in the Y-direction) to air-phase permeability in the row direction (in the X-direction).
- Note that YKRAT = 1.0 for isotropic conditions.
- A value for YKRAT is assigned to each geologic unit in the domain; the preprocessor assigns the value of YKRAT to all cells within the geologic unit.
- The input format is F5.0.

XKZ

- XKZ is input only if LTYPE = 1.
- XKZ is the air-phase permeability of a geologic unit in the Z-direction.
- The preprocessor assigns a value for XKZ to all cells in the geologic unit.
- XKZ is used to determine a vertical conductance between cell layers for use in MODFLOW.
- The physical units depend on IU1(7); the default is centimeters squared.
- The input format is E10.3.

AIRP

- AIRP is input only if LTYPE = 1 and ISS = 0.
- AIRP is the air-phase porosity of a geologic unit. The preprocessor assigns AIRP to all cells contained in the geologic unit.
- AIRP is used in the determination of the pneumatic storage coefficient required for transient simulations. Note that the preprocessor calculates storage coefficients internally, thus eliminating the need for the values to be input directly by the user.
- The input format is F5.0.

TRPY

- TRPY is input only if LTYPE = 2.
- TRPY is the ratio of air-phase permeability in the column direction (in the Y-direction) to air-phase permeability in the row direction (in the X-direction).

- Note that TRPY = 1.0 for isotropic conditions.
- TRPY is assigned for each cell layer.
- The input format is F10.0.

LOCAT
- LOCAT is input only if LTYPE = 2.
- LOCAT indicates the location of the data that will be put in the array. If LOCAT < 0, the sign is reversed to give the unit number from which an unformatted (binary) record will be read. If LOCAT = 0, every element in the array is set equal to the value CNSTNT. If LOCAT > 0, it is the unit number from which data values will be read in the format specified by FMTIN. Note that the preprocessor input file DATAIRx.PRE is assigned Fortran unit number 12 in PREAIR (LOCAT=12 for input from DATAIRx.PRE).
- The input format is I10.

CNSTNT
- CNSTNT is input only if LTYPE = 2.
- The use of CNSTNT depends on the value assigned to LOCAT. If LOCAT = 0, every element in the array is set equal to CNSTNT. If LOCAT ≠ 0, and if CNSTNT ≠ 0, every element in the array is multiplied by CNSTNT.
- The physical units depend on the item being input.
- The input format is F20.0.

FMTIN
- FMTIN is input only if LTYPE = 2.
- FMTIN is the format of the records containing the array values. It is used only if LOCAT > 0.
- Note that the format must be enclosed in parentheses, for example (6F10.3).
- The input format is 5A4.

IFLAG2
- IFLAG2 is input only if LTYPE = 2.
- IFLAG2 specifies the method of calculating vertical conductance for a layer.
- If IFLAG2 = 0, the program uses permeabilities and cell depths of two consecutive layers to determine the vertical conductances according to equation (51) in the MODFLOW manual. This is the most common setting. If IFLAG2 = 1, the program uses only the permeability and cell depth of a single cell layer to determine the vertical conductance according to equation (53) in the MODFLOW manual. This option is used only for a layer whose vertical permeability is significantly less than that of the layer beneath it.
- IFLAG2 defaults to a value of 0 if no value is specified.
- The input format is I10.

VPERM2(I,J)
- VEPERM2(I,J) are input only if LTYPE = 2.
- VPERM2(I,J) are the air-phase permeabilities in the Z-direction of each cell in a layer. The values for VPERM2(I,J) comprise a two-dimensional array, NCOL by NROW in size.
- The permeabilities are used to calculate vertical conductances in the model cells.

- The physical units depend on IU1(7); the default is centimeters squared.
- The input format is specified by FMTIN.

VCONT(I,J)

- VCONT(I,J) are input only if LTYPE = 2 and ISS=0.
- VCONT(I,J) are the air-phase porosities of each cell in a layer.
- Note that this definition does not correspond to the definition of VCONT(I,J) in the MODFLOW documentation. The values for VCONT(I,J) comprise a two-dimensional array, NCOL by NROW in size. The porosities are used in the determination of the pneumatic storage coefficient required for transient simulations.
- The input format is 4F10.0.

XPERM(I,J)

- XPERM(I,J) are input only if LTYPE = 2.
- XPERM(I,J) are the air permeabilities in the row direction (in the X-direction) of each cell in a model layer. The values for XPERM(I,J) comprise a two-dimensional array, NCOL by NROW in size.
- Note that XPERM is the same parameter as XKX for the case in which cell-by-cell definitions are desired (LTYPE = 2).
- The preprocessor multiplies XPERM by the cell depth (in the Z-direction) to obtain a transmissivity term.
- Air permeabilities in the column direction (in the Y-direction) are obtained by multiplying XPERM(I,J) by TRPY(I).
- The physical units depend on IU1(7); the default is centimeters squared.
- The input format is specified by FMTIN.

3.3.5 PREAIR Basic Output File BASAIRx.PRN

The preprocessor PREAIR outputs information directly to the file BASAIRx.PRN. The file name for the Basic Package output data is specified in the file INFILEx.PRE. The contents of BASAIRx.PRN are consistent with the format requirements used for input into MODFLOW.

BASAIRx.PRN file specifications are as follows:

Name of file:	Specified by user in file INFILEx.PRN (for example, BASAIR4.PRN).
File contents:	Simulation heading; number of layers, rows, columns, and stress periods; time units; package unit numbers; array selection; storage flags; boundary arrays; no-flow cell assignment; starting head arrays; simulation duration; number of time steps; time-step multiplier.
File application:	This preprocessor output file contains formatted data consistent with MODFLOW's Basic Package input file.

Fortran unit number: The program defines the output file as UNIT = 13.

Program output: Output is controlled in the subroutines SETUP and MODBAS. Output is written directly to the file.

Parameter units: All parameter units in the BASAIRx.PRN file have been converted to the cgs unit system by PREAIR.

The structure of BASAIRx.PRN and the format of the variables are given below. Fortran variables are defined at the end of this section.

1. Data: HEADING(32)
   Format: 20A4

2. Data: HEADING (continued)
   Format: 12A4

3. Data: NLAY NROW NCOL NPER ITMUNI
   Format: 4I10

4. Data: IUNIT(24)
   Format: 24I3
   (BCF WEL DRN RIV EVT XXX GHB RCH SIP XXX SOR OC)

5. Data: IAPART ISTRT
   Format: 2I10

Output items 6 and 7 (boundary array) once for each model layer.

6. Data: LOCAT,ICONST,FMTIN,IPRN
   Format: I10,F20.0,5A4,I10

Output item 7 as two-dimensional text array (IR=1,2,....,NROW).

7. Data: IBOUND(1,IR),IBOUND(2,IR),....,IBOUND(NCOL,IR)
   Format: FMTIN

8. Data: HNOFLO
   Format: F10.0

Output items 9 and 10 (starting pressure) once for each model layer.

9. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F20.0,5A4,I10

Output Item 10 as two-dimensional text array (IR=1,.,NROW).

10. Data: Shead(1,IR),Shead(2,IR),....,Shead(NCOL,IR)
    Format: FMTIN

Output Item 11 once for each stress period.

11. Data: PERLEN NSTP TSMULT
    Format: F10.0 I10 F10.0

An example of BASAIRx.PRN is given below:

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

1.    HEADING-------------------------------------3 DIMENSIONAL AIR FLOW ANALYSIS
2.    HEADING-------------------------------------5 ROWS, 7 COLS, 3 LAYS
3.    NLAY,NROW,NCOL,NPER,ITMUNI-----------------          4         5         7         1         1
4.    IUNIT(I)------------------------------------  7  0  0  0  0  0  0  0  8  0  0 11
5.    IAPART,ISTRT--------------------------------          0         1
6.    LOCAT,ICONST,FMTIN,IPRN------(u2dint)-------          1         1(20I3)                       0
7.    IBOUND(1,1),.,IBOUND(7,1)---(layer 1)--- -1 -1 -1 -1 -1 -1 -1
7.    IBOUND(1,2),.,IBOUND(7,2)---(layer 1)--- -1 -1 -1 -1 -1 -1 -1
7.    IBOUND(1,3),.,IBOUND(7,3)---(layer 1)--- -1 -1 -1 -1 -1 -1 -1
7.    IBOUND(1,4),.,IBOUND(7,4)---(layer 1)--- -1 -1 -1 -1 -1 -1 -1
7.    IBOUND(1,5),.,IBOUND(7,5)---(layer 1)--- -1 -1 -1 -1 -1 -1 -1
6.    LOCAT,ICONST,FMTIN,IPRN------(u2dint)-------          1         1(20I3)                       0
7.    IBOUND(1,1),.,IBOUND(7,1)---(layer 2)--- -2 -2 -2 -2 -2 -2 -2
7.    IBOUND(1,2),.,IBOUND(7,2)---(layer 2)--- -2  2  2  2  2  2 -2
7.    IBOUND(1,3),.,IBOUND(7,3)---(layer 2)--- -2  2  2  2  2  2 -2
7.    IBOUND(1,4),.,IBOUND(7,4)---(layer 2)--- -2  2  2  2  2  2 -2
7.    IBOUND(1,5),.,IBOUND(7,5)---(layer 2)--- -2 -2 -2 -2 -2 -2 -2
6.    LOCAT,ICONST,FMTIN,IPRN------(u2dint)-------          1         1(20I3)                       0
7.    IBOUND(1,1),.,IBOUND(7,1)---(layer 3)--- -3 -3 -3 -3 -3 -3 -3
7.    IBOUND(1,2),.,IBOUND(7,2)---(layer 3)--- -3  3  3  3  3  3 -3
7.    IBOUND(1,3),.,IBOUND(7,3)---(layer 3)--- -3  3  3 -3  3  3 -3
7.    IBOUND(1,4),.,IBOUND(7,4)---(layer 3)--- -3  3  3  3  3  3 -3
7.    IBOUND(1,5),.,IBOUND(7,5)---(layer 3)--- -3 -3 -3 -3 -3 -3 -3
```

Data item	Explanation (Continued)	1 5 10 15 20 25 30 35 40 45 50 55 60
6.	LOCAT,ICONST,FMTIN,IPRN———(u2dint)——	1 1(20I3) 0
7.	IBOUND(1,1),.,IBOUND(7,1)——(layer 4)——	-4 -4 -4 -4 -4 -4 -4
7.	IBOUND(1,2),.,IBOUND(7,2)——(layer 4)——	-4 4 4 4 4 4 -4
7.	IBOUND(1,3),.,IBOUND(7,3)——(layer 4)——	-4 4 4 4 4 4 -4
7.	IBOUND(1,4),.,IBOUND(7,4)——(layer 4)——	-4 4 4 4 4 4 -4
7.	IBOUND(1,5),.,IBOUND(7,5)——(layer 4)——	-4 -4 -4 -4 -4 -4 -4
8.	HNOFLO————————————————	.1027E+19
9.	LOCAT,CNSTNT,FMTIN,IPRN———(u2drel)——	1 1.000(4E15.8) 0
10.	Shead(1,1),.,Shead(4,1)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,1),.,Shead(7,1)———(layer 1)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,2),.,Shead(4,2)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,2),.,Shead(7,2)———(layer 1)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,3),.,Shead(4,3)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,3),.,Shead(7,3)———(layer 1)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,4),.,Shead(4,4)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,4),.,Shead(7,4)———(layer 1)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,5),.,Shead(4,5)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,5),.,Shead(7,5)———(layer 1)——	.10265742E+13 .10265742E+13 .10265742E+13
9.	LOCAT,CNSTNT,FMTIN,IPRN———(u2drel)——	1 1.000(4E15.8) 0
10.	Shead(1,1),.,Shead(4,1)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,1),.,Shead(7,1)———(layer 2)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,2),.,Shead(4,2)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,2),.,Shead(7,2)———(layer 2)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,3),.,Shead(4,3)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,3),.,Shead(7,3)———(layer 2)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,4),.,Shead(4,4)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,4),.,Shead(7,4)———(layer 2)——	.10265742E+13 .10265742E+13 .10265742E+13
10.	Shead(1,5),.,Shead(4,5)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,5),.,Shead(7,5)———(layer 2)——	.10265742E+13 .10265742E+13 .10265742E+13
9.	LOCAT,CNSTNT,FMTIN,IPRN———(u2drel)——	1 1.000(4E15.8) 0
10.	Shead(1,1),.,Shead(4,1)————————	.10265742E+13 .10265742E+13 .10265742E+13 .10265742E+13
	Shead(5,1),.,Shead(7,1)———(layer 3)——	.10265742E+13 .10265742E+13 .10265742E+13

Data item	Explanation (Continued)	1 5 10 15	20 25 30	35 40 45	50 55 60
10.	Shead(1,2),.,Shead(4,2)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,2),.,Shead(7,2)——(layer 3)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,3),.,Shead(4,3)——	.10265742E+13	.10265742E+13	.10265742E+13	.83152513E+12
	Shead(5,3),.,Shead(7,3)——(layer 3)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,4),.,Shead(4,4)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,4),.,Shead(7,4)——(layer 3)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,5),.,Shead(4,5)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,5),.,Shead(7,5)——(layer 3)——	.10265742E+13	.10265742E+13	.10265742E+13	
9.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	1	1.000(4E15.8)		0
10.	Shead(1,1),.,Shead(4,1)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,1),.,Shead(7,1)——(layer 4)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,2),.,Shead(4,2)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,2),.,Shead(7,2)——(layer 4)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,3),.,Shead(4,3)——	.10265742E+13	.10265742E+13	.10265742E+13	.92648325E+12
	Shead(5,3),.,Shead(7,3)——(layer 4)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,4),.,Shead(4,4)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,4),.,Shead(7,4)——(layer 4)——	.10265742E+13	.10265742E+13	.10265742E+13	
10.	Shead(1,5),.,Shead(4,5)——	.10265742E+13	.10265742E+13	.10265742E+13	.10265742E+13
	Shead(5,5),.,Shead(7,5)——(layer 4)——	.10265742E+13	.10265742E+13	.10265742E+13	
11.	PERLEN,NSTP,TSMULT——	3600.	1 1.		

The definitions of selected variables included in the output file BASAIRx.PRN are presented below. This section deals primarily with variables that were specified or redefined for the air-flow simulation. Variables are presented in the order in which they appear in the data file and have been standardized to a cgs unit system by the preprocessor. Information on variables not discussed below can be found in Section 3.3.4 or in the MODFLOW documentation.

ITMUNI

- ITMUNI indicates the time unit for the model data. The definition is the same as that for ITMUNI in the MODFLOW documentation.
- ITMUNI is specified within the preprocessor code and is defaulted to a value of 1 (time units of seconds). The setting is consistent with the default unit system used in the preprocessor.

IUNIT(I)

- IUNIT(I) is the input unit number to be used by the major package options. The settings are described in the MODFLOW documentation. Apart from the SIP or SOR packages, all settings are defaulted within the program as follows:
  - The Block-Centered-Flow Package is assigned a unit number = 7. The Block-Centered-Flow Package is always required.
  - The Well Package is not used in pneumatic simulations. Constant-pressure cells are used to model well and trench boundary conditions as discussed in Section 3.1.3.
  - The Drain, River, Evapotranspiration, and Recharge Packages are not used for pneumatic simulations.
  - The SIP package is assigned a unit number = 8 (if selected). The Strongly Implicit Procedure matrix solver is required if the SOR option is not specified.
  - The SOR package is assigned a unit number = 9 (if selected). The Slice Successive Overrelaxation matrix solution method is required if the SIP option is not specified.
  - The Output-Control Package is assigned a unit number = 11. The Output-Control Package is always required.
- IUNIT(I) is specified within the preprocessor code and is defaulted to the above settings. Packages not required are assigned a unit number of zero.

IAPART

- IAPART indicates whether the array BUFF is separate from (if IAPART=1), or occupies the same space as the array RHS (if IAPART=0). The definition is the same as that for IAPART in the MODFLOW documentation.
- IAPART is specified within the preprocessor code and is defaulted to a value of 0 (BUFF and RHS occupy the same space).

ISTRT

- ISTRT indicates whether starting heads are to be saved (0) or discarded (1). The definition is the same as for IAPART in the MODFLOW documentation.
- ISTRT is specified within the preprocessor code and is defaulted to a value of 0 (starting heads are not saved).

IBOUND(NCOL,NROW)

- IBOUND is the array defining node types in each layer. Boundary cells (other than those representing wells and trenches) are specified as constant-head cells at atmospheric pressure squared. All well and trench cells are specified as constant-head cells at well/trench pressures squared. All cells directly above the well screen and extending to the surface are specified as inactive to simulate well casing. All interior cells are specified as active. An additional cell layer (layer 0) also is superimposed on the model domain; these cells are set to a constant head at atmospheric pressure squared (see section 3.1.3). IBOUND(NCOL,NROW) is defined in the MODFLOW documentation.
- IBOUND is specified within the preprocessor code for each cell layer. Active cells are assigned positive values. Constant-head cells are assigned negative values. Inactive cells are assigned zero values. The user can force the cells in the domain to act as no-flow cells by setting permeability values in the no-flow cells to zero.

HNOFLO

- HNOFLO is the value of the head to be assigned to all inactive cells throughout simulation. The definition is the same as that for HNOFLO in the MODFLOW documentation.
- HNOFLO is specified within the preprocessor code and is defaulted to a value of 0.1027E+19, which reduces to a value of approximately 1,000.0 when the postprocessor POSTAIR applies the air-flow transformations to head output from MODFLOW ($(0.1027E+19)^{1/2}/1{,}013{,}250.0 \approx 1000.0$).

SHEAD(NCOL,NROW)

- SHEAD is the pressure squared at the start of the simulation. In general, the initial conditions in the domain are equal to the atmospheric pressure squared. SHEAD is defined in a similar way to SHEAD in the MODFLOW documentation, in which pressure squared replaces head.
- SHEAD is generated in the preprocessor from the values specified by the user for atmospheric pressure and well/trench pressure.

3.3.6 PREAIR Output-Control File OCAIRx.PRN

The preprocessor PREAIR outputs information directly to the file OCAIRx.PRN. The name of the Output Control Package file is specified in the file INFILEx.PRE. The contents of the file are consistent with the format requirements used for input of Output Control information into MODFLOW.

OCAIRx.PRN file specifications are as follows:

Name of file:	Specified by the user in the file INFILEx.PRN (for example, OCAIR4.PRN)
File contents:	Format codes for head and drawdown printout, unit numbers for head and drawdown output, head and drawdown output codes, printout flags for volumetric budget, cell-by-cell flow, head terms, and drawdown terms, and flags to save head and drawdowns.
File application:	This preprocessor output file contains formatted data consistent with MODFLOW's Output Control input file.
Fortran unit number:	The program defines the output file as UNIT = 14.
Program output:	Output is controlled in the subroutine MODOC.
Parameter units:	The contents of this file control MODFLOW operations. All output is dimensionless.

The structure of OCAIRx.PRN is as follows:

1. Data: IHEDFM IDDNFM IHEDUN IDDNUN
   Format: 4I10

Output item 2 and 3 once for each time step.

2. Data: INCODE IHDDFL IBUDFL ICBCFL
   Format: 4I10

3. Data: IHDPR IDDPR IHDSV IDDSV
   Format: 4I10

An example of OCAIRx.PRN is given below:

Data item	Explanation	Input records 1–10	11–20	21–30	31–40
1.	IHEDFM,IDDNFM,IHEDUN,IDDNUN	0	0	12	0
2.	INCODE,IHDDFL,IBUDFL,ICBCFL	0	1	0	1
3.	IHDPR,IDDPR,IHDSV,IDDSV	0	0	1	0

The definitions of the variables included in the output file OCAIRx.PRN are presented below. Because all the settings in OCAIRx.PRN are defined internally within the preprocessor code, the following section presents the default settings. Note that head output from MODFLOW is used to obtain pressure values in the domain. In the following discussion, keep in mind that pressure data reside in what is referred to as head output.

IHEDFM

- IHEDFM is a format code for head (pressure) output sent to the MODFLOW text file. Note, however, that only values sent to binary files are used by the postprocessor and any setting for IHEDFM can be specified.
- IHEDFM defaults to a value of 0 and is set within the preprocessor.

IDDNFM

- IDDNFM is a format code for drawdown output sent to the MODFLOW text file. Note, however, that only values sent to binary files are used by the postprocessor and any setting for IDDNFM can be used. IDDNFM is defined in the MODFLOW documentation.
- IDDNFM defaults to a value of 0 and is set within the preprocessor.

IHEDUN
- IHEDUN is the unit number to which head (pressure) output is written if it is saved on disk. IHEDUN is defined in the MODFLOW documentation.
- IHEDUN defaults to a value of 12 (save head output to disk) and is set within the preprocessor.

IDDNUN
- IDDNUN is the unit number to which drawdowns are written if they are saved on disk. IDDNUN is defined in the MODFLOW documentation.
- IDDNUN defaults to a value of 0 (unit number) and is set within the preprocessor.

INCODE
- INCODE is the head/drawdown output code. Its value determines whether layer-by-layer specifications from the last time step are used (INCODE<0), all layers are treated in the same way (INCODE=0), or one record is specified for each layer (INCODE>0). INCODE is defined in the MODFLOW documentation.
- INCODE defaults to a value of 0 (all layers are treated in the same way) and is specified within the preprocessor.

IHDDFL
- IHDDFL is the head/drawdown output flag. Its value determines whether heads and drawdown output are saved/printed (IHDDFL>0) or discarded (IHDDFL=0). IHDDFL is defined in the MODFLOW documentation.
- IHDDFL defaults to a value of 1 (heads and drawdowns are saved according to the flags set in item 3) and is specified within the preprocessor. Note that this setting must be specified to generate binary output.

IBUDFL
- IBUDFL is the budget print flag. Its value determines whether the overall volumetric budget is printed (IBUDFL>0) or not (IBUDFL=0). IBUDFL is defined in the MODFLOW documentation.
- IBUDFL defaults to a value of 0 (volumetric budget is not printed) and is set within the preprocessor. Note that the overall volumetric budget always is printed in the text output file at the end of a stress period, even if the value of IBUDFL is zero; however, such output values must be transformed to dimensionally correct air-flow terms prior to analyses.

ICBCFL
- ICBCFL is a cell-by-cell flow-term flag. Its value determines whether cell-by-cell flow terms are printed/saved on disk (ICBCFL>0) or not (ICBCFL=0). ICBCFL is defined in the MODFLOW documentation.
- ICBCFL defaults to a value of 1 (cell-by-cell flow terms are printed/saved according to the settings specified in the Block-Centered-Flow package) and is specified within the preprocessor. Note that a value must be specified to generate binary output.

IHDPR

- IHDPR is the output flag for head (pressure) printout. Its value determines whether head for the corresponding layer is printed (IHDPR>0) or not (IHDPR=0). The definition for IHDPR is the same as that for HDPR in the MODFLOW documentation.
- IHDPR defaults to a value of 0 (head is not printed to the text output file) and is specified within the preprocessor. Note that this setting does not affect the binary head output.

IDDPR

- IDDPR is the output flag for drawdown printout. Its value determines whether drawdown for the corresponding layer is printed (IDDPR>0) or not (IDDPR=0). The definition for IDDPR is the same as that for DDPR in the MODFLOW documentation.
- IDDPR is defaulted to a value of 0 (drawdown is not printed) and is specified within the preprocessor.

IHDSV

- IHDSV is the output flag for saving head (pressure). Its value determines whether head for the corresponding layer is saved (IHDSV>0) or not (IHDSV=0). The definition for IHDSV is the same as that for Hdsv in the MODFLOW documentation.
- IHDSV defaults to a value of 1 (head is saved) and is specified within the preprocessor.

IDDSV

- IDDSV is the output flag for saving drawdown. Its value determines whether drawdown for the corresponding layer is saved (IDDSV>0) or not (IDDSV=0). The definition of IDDSV is the same as that for Ddpr in the MODFLOW documentation.
- IDDSV defaults to a value of 0 and is specified within the preprocessor.

3.3.7 PREAIR Block-Centered-Flow Output File BCFAIRx.PRN

The preprocessor PREAIR outputs information directly to the file BCFAIRx.PRN. The file name for the Block-Centered-Flow (BCF) Package output data is specified in the file INFILEx.PRE. The contents of the file are consistent with the format requirements used for input of block-centered-flow information into MODFLOW. The following discusses a typical Block-Centered-Flow output file and values of parameters used to make the output compatible with both MODFLOW and the pneumatic model requirements.

BCFAIRx.PRN file specifications are as follows:

Name of file:	Specified by the user in the file INFILEx.PRN (for example, BCFAIR4.PRN).
File contents:	Steady-state or transient simulation, unit number for binary flow output, layer specification, anisotropy factors, row and column cell widths, storage factors, transmissivity, vertical conductance.
File application:	This preprocessor output file contains formatted data consistent with MODFLOW's Block-Centered-Flow Package input file.

Fortran unit number: The program defines the output file as UNIT = 15.

Program output: Output is controlled in the subroutine MODBCF. Output is written directly to the file.

Parameter units: All parameter units in the BCFAIRx.PRN file have been converted to the cgs unit system by PREAIR.

The structure of BCFAIRx.PRN is as follows:

1. Data: ISS IBCFCB
   Format: 2I10

   Output item 2 (layer type) once for each 40 or fewer layers.
2. Data: LAYCON(NLAY) (Maximum of 80 layers)
   Format: 40I2

   Output items 3 and 4 (anisotropy ratios) for each model layer.
3. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F20.0,5A4,I10

   Output item 4 as text array (IL=1,2,...,NLAY).
4. Data: TRPY(IL)
   Format: FMTIN

   Output items 5 and 6 (cell width along rows) for each model column.
5. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F20.0,5A4,I10

   Output item 6 as text array (IC=1,2,...,NCOL).
6. Data: DELR(IC)
   Format: FMTIN

   Output items 7 and 8 (cell width along columns) for each model row.
7. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F20.0,5A4,I10

   Output item 8 as text array (IR=1,2,...,NROW).
8. Data: DELC(IR)
   Format: FMTIN

   A subset of the MODFLOW two-dimensional arrays is used to describe each layer. The subset for an air-flow simulation always comprises input for transmissivity (Tran) and vertical conductance (Vcont) in each layer because LAYCON=0 is fixed. Input for the pneumatic storage coefficient, sfl(NCOL,NROW), in each layer is entered only if the simulation is transient (ISS=0). Again, because LAYCON=0 is fixed for air-flow simulations, no input is required for the hydraulic conductivity (HY), aquifer-bottom (BOT) and top (TOP) elevation, or secondary-storage-factor (sf2) arrays. All of the arrays (items 9-14) for layer 1 are output first, then all of the arrays for layer 2 are output, and so on, as is done in MODFLOW. If input parameters are constant within a particular layer, the abbreviated form (LOCAT = 0) can be used and the array input can be skipped. For variable parameters, values at each cell in two-dimensional text arrays (for LOCAT > 0) or two-dimensional binary arrays (for LOCAT < 0) must be defined.

If ISS=0 (transient simulation) then INPUT items 9 and 10 (air-phase storage coefficient); omit if ISS ≠ 0.

9. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F10.0,5A4,I10

IF LOCAT > 0 (that is, nonuniform air-phase storage coefficient) then input item 10 as a two-dimensional text array (IR=1,.,NROW); omit if LOCAT = 0.

10a. Data: sfl(1,IR),sfl(2,IR),.....,sfl(NCOL,IR)
   Format: FMTIN

If LOCAT < 0 (nonuniform air-phase storage coefficient) then input item 10 as two-dimensional binary data (IR=1,...,NROW); omit if LOCAT = 0.

10b. Data: sfl(1,IR),sfl(2,IR),.....,sfl(NCOL,IR)
   Format: binary

Input items 11 and 12 (air phase transmissivity).

11. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F10.0,5A4,I10

If LOCAT > 0 (nonuniform air-phase transmissivity) then input item 12 as a two-dimensional text array (IR=1,.,NROW); omit if LOCAT = 0.

12a. Data: Tran(1,IR),Tran(2,IR),.....,Tran(NCOL,IR)
   Format: FMTIN

If LOCAT < 0 (nonuniform air-phase transmissivity) then input item 12 as two-dimensional binary data (IR=1,,NROW); omit if LOCAT = 0.

12b. Data: Tran(1,IR),Tran(2,IR),.....,Tran(NCOL,IR)
   Format: binary

Input items 13 and 14 (air-phase vertical conductance).

13. Data: LOCAT,CNSTNT,FMTIN,IPRN
   Format: I10,F10.0,5A4,I10

If LOCAT > 0 (non-uniform air-phase vertical conductance) then input item 14 as a two-dimensional text array (IR=1,.,NROW); omit if LOCAT = 0.

14a. Data: Vcont(1,IR),Vcont(2,IR),.....,Vcont(NCOL,IR)
Format: FMTIN

If LOCAT < 0 (nonuniform air-phase vertical conductance) then input item 14 as two-dimensional binary data (IR=1,,NROW); omit if LOCAT = 0.

14b. Data: Vcont(1,IR),Vcont(2,IR),.....,Vcont(NCOL,IR)
Format: binary

An example of BCFAIRx.PRN is given below:

Data item	Explanation	Input records (columns 1 5 10 15 20 25 30 35 40 45 50 55 60)					
1.	ISS,IBCFCB	1	13				
2.	LAYCON(NLAY)	0 0 0 0					
3.	LOCAT,CNSTNT,FMTIN,IPRN——(u1drel)	7	1.000(6F10.3)			0	
4.	TRPY(1),..,TRPY(4)——(layer 1)	1.000	1.000	1.000	1.000		
5.	LOCAT,CNSTNT,FMTIN,IPRN——(u1drel)	7	1.000(6F10.3)			0	
6.	DELR(1),..,DELR(6)——(col 1..6)	100.000	100.000	100.000	100.000	100.000	100.000
6.	DELR(7)——(col 7)	100.000					
7.	LOCAT,CNSTNT,FMTIN,IPRN——(u1drel)	7	1.000(6F10.3)			0	
8.	DELC(1),..,DELC(5)——(row 1..5)	100.000	100.000	100.000	100.000	100.000	
11.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)	7	1.000(4E15.8)			0	
12a.	TRAN(1,1),.......,TRAN(4,1)	.10000000E+01	.10000000E+01	.10000000E+01	.10000000E+01		
	TRAN(5,1),...,TRAN(7,1)——(layer 1)	.10000000E+01	.10000000E+01	.10000000E+01			
12a.	TRAN(1,2),.......,TRAN(4,2)	.10000000E+01	.10000000E+01	.10000000E+01	.10000000E+01		
	TRAN(5,2),...,TRAN(7,2)——(layer 1)	.10000000E+01	.10000000E+01	.10000000E+01			
12a.	TRAN(1,3),.......,TRAN(4,3)	.10000000E+01	.10000000E+01	.10000000E+01	.10000000E+01		
	TRAN(5,3),...,TRAN(7,3)——(layer 1)	.10000000E+01	.10000000E+01	.10000000E+01			
12a.	TRAN(1,4),.......,TRAN(4,4)	.10000000E+01	.10000000E+01	.10000000E+01	.10000000E+01		
	TRAN(5,4),...,TRAN(7,4)——(layer 1)	.10000000E+01	.10000000E+01	.10000000E+01			
12a.	TRAN(1,5),.......,TRAN(4,5)	.10000000E+01	.10000000E+01	.10000000E+01	.10000000E+01		
	TRAN(5,5),...,TRAN(7,5)——(layer 1)	.10000000E+01	.10000000E+01	.10000000E+01			

Data item	Explanation (Continued)	1 5 10 15	20 25 30	35 40 45	50 55 60
13.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
14a.	VCONT(1,1),.....,VCONT(4,1)——————	.50000000E-08	.50000000E-08	.50000000E-08	.50000000E-08
	VCONT(5,1),...,VCONT(7,1)——(layer 1)——	.50000000E-08	.50000000E-08	.50000000E-08	
14a.	VCONT(1,2),.....,VCONT(4,2)——————	.50000000E-08	.50000000E-08	.50000000E-08	.50000000E-08
	VCONT(5,2),...,VCONT(7,2)——(layer 1)——	.50000000E-08	.50000000E-08	.50000000E-08	
14a.	VCONT(1,3),.....,VCONT(4,3)——————	.50000000E-08	.50000000E-08	.50000000E-08	.50000000E-08
	VCONT(5,3),...,VCONT(7,3)——(layer 1)——	.50000000E-08	.50000000E-08	.50000000E-08	
14a.	VCONT(1,4),.....,VCONT(4,4)——————	.50000000E-08	.50000000E-08	.50000000E-08	.50000000E-08
	VCONT(5,4),...,VCONT(7,4)——(layer 1)——	.50000000E-08	.50000000E-08	.50000000E-08	
14a.	VCONT(1,5),.....,VCONT(4,5)——————	.50000000E-08	.50000000E-08	.50000000E-08	.50000000E-08
	VCONT(5,5),...,VCONT(7,5)——(layer 1)——	.50000000E-08	.50000000E-08	.50000000E-08	
11.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
12a.	TRAN(1,1),.......,TRAN(4,1)——————	.10000000E-05	.10000000E-05	.10000000E-05	.10000000E-05
	TRAN(5,1),...,TRAN(7,1)——(layer 2)——	.10000000E-05	.10000000E-05	.10000000E-05	
12a.	TRAN(1,2),.......,TRAN(4,2)——————	.10000000E-05	.10000000E-05	.10000000E-05	.10000000E-05
	TRAN(5,2),...,TRAN(7,2)——(layer 2)——	.10000000E-05	.10000000E-05	.10000000E-05	
12a.	TRAN(1,3),.......,TRAN(4,3)——————	.10000000E-05	.10000000E-05	.10000000E-05	.10000000E-05
	TRAN(5,3),...,TRAN(7,3)——(layer 2)——	.10000000E-05	.10000000E-05	.10000000E-05	
12a.	TRAN(1,4),.......,TRAN(4,4)——————	.10000000E-05	.10000000E-05	.10000000E-05	.10000000E-05
	TRAN(5,4),...,TRAN(7,4)——(layer 2)——	.10000000E-05	.10000000E-05	.10000000E-05	
12a.	TRAN(1,5),.......,TRAN(4,5)——————	.10000000E-05	.10000000E-05	.10000000E-05	.10000000E-05
	TRAN(5,5),...,TRAN(7,5)——(layer 2)——	.10000000E-05	.10000000E-05	.10000000E-05	
13.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
14a.	VCONT(1,1),.....,VCONT(4,1)——————	.13333333E-10	.13333333E-10	.13333333E-10	.13333333E-10
	VCONT(5,1),...,VCONT(7,1)——(layer 2)——	.13333333E-10	.13333333E-10	.13333333E-10	
14a.	VCONT(1,2),.....,VCONT(4,2)——————	.13333333E-10	.13333333E-10	.13333333E-10	.13333333E-10
	VCONT(5,2),...,VCONT(7,2)——(layer 2)——	.13333333E-10	.13333333E-10	.13333333E-10	
14a.	VCONT(1,3),.....,VCONT(4,3)——————	.13333333E-10	.13333333E-10	.13333333E-10	.13333333E-10
	VCONT(5,3),...,VCONT(7,3)——(layer 2)——	.13333333E-10	.13333333E-10	.13333333E-10	
14a.	VCONT(1,4),.....,VCONT(4,4)——————	.13333333E-10	.13333333E-10	.13333333E-10	.13333333E-10
	VCONT(5,4),...,VCONT(7,4)——(layer 2)——	.13333333E-10	.13333333E-10	.13333333E-10	
14a.	VCONT(1,5),.....,VCONT(4,5)——————	.13333333E-10	.13333333E-10	.13333333E-10	.13333333E-10
	VCONT(5,5),...,VCONT(7,5)——(layer 2)——	.13333333E-10	.13333333E-10	.13333333E-10	

Data item	Explanation (Continued)	1 5 10 15	20 25 30	35 40 45	50 55 60
11.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
12a.	TRAN(1,1),.......,TRAN(4,1)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,1),...,TRAN(7,1)——(layer 3)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,2),.......,TRAN(4,2)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,2),...,TRAN(7,2)——(layer 3)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,3),.......,TRAN(4,3)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,3),...,TRAN(7,3)——(layer 3)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,4),.......,TRAN(4,4)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,4),...,TRAN(7,4)——(layer 3)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,5),.......,TRAN(4,5)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,5),...,TRAN(7,5)——(layer 3)——	.20000000E-05	.20000000E-05	.20000000E-05	
13.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
14a.	VCONT(1,1),.....,VCONT(4,1)————	.20000000E-10	.20000000E-10	.20000000E-10	.20000000E-10
	VCONT(5,1),...,VCONT(7,1)—(layer 3)——	.20000000E-10	.20000000E-10	.20000000E-10	
14a.	VCONT(1,2),.....,VCONT(4,2)————	.20000000E-10	.20000000E-10	.20000000E-10	.20000000E-10
	VCONT(5,2),...,VCONT(7,2)—(layer 3)——	.20000000E-10	.20000000E-10	.20000000E-10	
14a.	VCONT(1,3),.....,VCONT(4,3)————	.20000000E-10	.20000000E-10	.20000000E-10	.20000000E-10
	VCONT(5,3),...,VCONT(7,3)—(layer 3)——	.20000000E-10	.20000000E-10	.20000000E-10	
14a.	VCONT(1,4),.....,VCONT(4,4)————	.20000000E-10	.20000000E-10	.20000000E-10	.20000000E-10
	VCONT(5,4),...,VCONT(7,4)—(layer 3)——	.20000000E-10	.20000000E-10	.20000000E-10	
14a.	VCONT(1,5),.....,VCONT(4,5)————	.20000000E-10	.20000000E-10	.20000000E-10	.20000000E-10
	VCONT(5,5),...,VCONT(7,5)—(layer 3)——	.20000000E-10	.20000000E-10	.20000000E-10	
11.	LOCAT,CNSTNT,FMTIN,IPRN——(u2drel)——	7	1.000(4E15.8)		0
12a.	TRAN(1,1),.......,TRAN(4,1)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,1),...,TRAN(7,1)——(layer 4)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,2),.......,TRAN(4,2)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,2),...,TRAN(7,2)——(layer 4)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,3),.......,TRAN(4,3)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,3),...,TRAN(7,3)——(layer 4)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,4),.......,TRAN(4,4)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,4),...,TRAN(7,4)——(layer 4)——	.20000000E-05	.20000000E-05	.20000000E-05	
12a.	TRAN(1,5),.......,TRAN(4,5)————	.20000000E-05	.20000000E-05	.20000000E-05	.20000000E-05
	TRAN(5,5),...,TRAN(7,5)——(layer 4)——	.20000000E-05	.20000000E-05	.20000000E-05	

The definitions of selected variables included in the output file BCFAIRx.PRN are presented below. This section deals primarily with variables that are specified or redefined for the air-flow simulation. Variables are presented in the order in which they appear in the data file and have been standardized to the cgs unit system by the preprocessor. Information on variables not discussed below can be found in Section 3.3.4 or in the MODFLOW documentation.

IBCFCB

- IBCFCB is a flag and unit number for printing or recording cell-by-cell flow terms. Its value determines whether flow terms are recorded in a file with a Fortran unit number specified by IBCFCB > 0. Flow terms are not be saved or printed if IBCFCB = 0. Constant-head flow terms are printed if IBCFCB < 0.
- IBCFCB is defaulted to a value of 13 (record flow terms to a binary file defined by IBCFCB) and is specified within the preprocessor. This value must be specified to generate binary flow output.

LAYCON(NLAY)

- LAYCON is the specified layer type for each layer. A value of 0 is used to identify a confined layer. A value of 1 specifies a layer unconfined and values of 2 and 3 are used to identify layers that can change between confined and unconfined. For confined layers, flow parameters such as transmissivity and storage coefficient are constant during the simulation. Because this condition also is imposed on the air-flow equation when developed, a LAYCON value of 0 applies to all air-flow simulations regardless of the geologic properties of the domain.
- LAYCON is defaulted to a value of 0 for each layer (confined layers) and is specified within the preprocessor.

TRPY(NLAY)

- TRPY is a one-dimensional array that contains an anisotropy factor for each layer. TRPY is the ratio of the pneumatic equivalent of transmissivity along a column (in the Y-direction) to the pneumatic equivalent of transmissivity along a row (in the X-direction). Note that the pneumatic equivalent of transmissivity is the product of air- phase intrinsic permeability (cm^2) and cell depth (cm). One value per layer is required and must be input in accordance with MODFLOW utility module U1DREL requirements. For isotropic conditions, TRPY = 1.0. The definition of TRPY is similar to that in the MODFLOW documentation.
- TRPY is required to implement MODFLOW and is specified by the user.

DELR(NCOL)

- DELR is a one-dimensional array that contains cell widths along rows. One value per column is required and must be input in accordance with MODFLOW utility module U1DREL requirements.

DELC(NROW)

- DELC is a one-dimensional array that contains cell widths along columns. One value per row is required and must be input in accordance with MODFLOW utility module U1DREL requirements.
- DELC(NROW) is required to implement MODFLOW and is specified by the user.

sf1(NCOL,NROW)

- sf1 is a two-dimensional array that contains the pneumatic equivalents of storage coefficients and consists of the following expression: (the air-filled porosity) * (the depth of the model cell) * (air phase viscosity at air temperature)/(air pressure). The storage values must be calculated and specified at each cell location in the model domain for transient simulations.
- sf1() is only specified for transient simulations.

Tran(NCOL,NROW)

- Tran is a two-dimensional array that contains pneumatic equivalents of transmissivity. Note that the pneumatic equivalent of transmissivity is the product of air-phase intrinsic permeability (cm^2) along rows (in the X-direction) and the cell depth (cm). The transmissivity values must be calculated and specified at each cell location in the model domain for all simulations.
- Tran must be specified for all simulations by the user.

Vcont(NCOL,NROW)

- Vcont is a two-dimensional array that contains pneumatic equivalents of vertical conductance. Note that a number of options is available in the MODFLOW documentation for determining the pneumatic equivalent of vertical conductance. In general, the terms involve some combination of the quotient of the air-phase intrinsic permeability (cm^2) in the Z-direction and the cell depth (cm). The vertical-conductance values must be calculated and specified at each cell location in the model domain for all simulations. Vcont is the pneumatic equivalent of the Vcont array defined in the MODFLOW documentation.
- Vcont must be specified for all simulations by the user.

3.3.8 PREAIR Strongly Implicit Package and Successive Overrelaxation Output Files SIPAIRx.PRN and SORAIRx.PRN

The preprocessor PREAIR outputs information directly to the file SIPAIRx.PRN (for the SIP option) or SORAIRx.PRN (for the SOR option). The matrix-solver option is specified in the file INFILEx.PRE. The contents of the file are consistent with the format requirements used for input of the matrix-solver information into MODFLOW. The following discussion includes examples of SIP and SOR files and indicates values of parameters used to make the output compatible with both MODFLOW and the pneumatic model.

SIPAIRx.PRN and SORAIRx.PRN file specifications are as follows:

Name of file:	Specified by the user in the file INFILEx.PRN (for example, SIPAIR4.PRN or SORAIR4.PRN).
File contents:	Maximum number of iterations, number of iteration parameters to be used (SIP only), acceleration factor, head-change criteria for convergence, flag for iteration parameter seed (SIP only), iteration seed value (SIP only), printout interval for SIP or SOR.

File application:	This preprocessor output file contains formatted data consistent with MODFLOW's SIP or SOR input files.
Fortran unit number:	The program defines the output file as UNIT = 16.
Program output:	Output is controlled in the subroutine MODSIP.

The structure of SIPAIRx.PRN is as follows:

1. Data: MXITER NPARM
   Format: 2I10

2. Data: ACCL HCLOSE IPCALC WSEED IPRSIP
   Format: F10.0,F10.0,3I10

The structure of SORAIRx.PRN is as follows:

1. Data: MXITER
   Format: I10

2. Data: ACCL HCLOSE IPSOR
   Format: F10.0,F10.0,I10

An example of SIPAIRx.PRN is given below:

Data item	Explanation	Input Records 1	5	10	15	20	25	30	35	40	45	50
1.	MXITER,NPARM			100		5						
2.	ACCL,HCLOSE,IPCALC,WSEED,IPRSIP			1.0		100.0		1				100

An example of SORAIRx.PRN is given below:

Data item	Explanation	Input Records 1	5	10	15	20	25	30	35	40	45	50
1.	MXITER			100								
2.	ACCL,HCLOSE,IPRSOP			1.0		100.0		100				

The definitions of variables included in the output files SIPAIRx.PRN and SORAIRx.PRN are presented below.

MXITER

- MXITER is the maximum number of iterations allowed in one time step before MODFLOW terminates. MXITER is defined in the MODFLOW documentation.
- MXITER defaults to a value of 100 and is specified within the preprocessor code.

NPARM (SIP only)

- NPARM is the number of iteration parameters to be used. NPARM is defined in the MODFLOW documentation.
- NPARM defaults to a value of 5 (as recommended in the MODFLOW documentation) and is specified within the preprocessor.

ACCL

- ACCL is the acceleration parameter. ACCL is defined in the MODFLOW documentation.
- ACCL defaults to a value of 1.0 (as recommended in the MODFLOW documentation) and is specified within the preprocessor.

HCLOSE

- HCLOSE is the head-change criterion for convergence. In air-flow simulations, MODFLOW tests the change in the air-pressure-squared term at each node during an iteration. When this value is less than or equal to HCLOSE, iteration stops. The definition of HCLOSE is essentially the same as that for HCLOSE in the MODFLOW documentation except that changes in pressure squared are used rather than changes in hydraulic head.
- HCLOSE defaults to a value of 100.0. This value is larger than that typically used for a ground-water-flow simulation using MODFLOW because typical values of pressure squared are of the order 1×10^{12}. This default value can require adjustments for certain air-flow simulations. HCLOSE is specified within the preprocessor.

IPCALC (SIP only)

- IPCALC is a flag that indicates the source of the iteration parameter seed. Its value determines whether the seed will be entered by the user (IPCALC = 0) or calculated at the start of the simulation from problem parameters (IPCALC = 1). IPCALC is defined in the MODFLOW documentation.
- IPCALC defaults to a value of 1 and is specified within the preprocessor.

WSEED (SIP only)

- WSEED is the actual value of the seed. WSEED is required only if IPCALC = 0. WSEED is defined in the MODFLOW documentation.

IPRSIP (for SIP) or IPRSOR (for SOR)

- IPRSIP or IPRSOR is the printout interval for SIP or SOR. IPRSIP and IPRSOR are defined in the MODFLOW documentation.
- IPRSIP or IPRSOR defaults to a value of 100 and is specified within the preprocessor.

3.3.9 PREAIR Input File INFILE.MOD

The preprocessor PREAIR outputs information directly to the file INFILE.MOD. The name of the MODFLOW input file listing is specified within the preprocessor. The contents of the file comprise MODFLOW input and output file names. The file can be used either directly when implementing MODFLOW on a personal computer or as a file summary when using MODFLOW on an alternate computing system. The following discussion presents an example of the INFILE.MOD file.

INFILE.MOD file specifications are as follows:

Name of file:	Specified within PREAIR (for example, INFILE.MOD)
File contents:	MODFLOW text output file name, MODFLOW Basic input file name, MODFLOW Block-Centered-Flow input file name, MODFLOW Matrix-Solver input file name, MODFLOW Output-Control input file name, MODFLOW binary head output-file name, MODFLOW binary flow output-file name.
File application:	This preprocessor output file contains a listing of file names used when running MODFLOW.
Fortran unit number:	The program defines the output file as UNIT = 20.
Program output:	Output is controlled in the subroutine SETUP. Output is written directly to the file.

The structure of INFILE.MOD is as follows:

1. Data: FNAME(12)
   Format: A12

2. Data: FNAME(3)
   Format: A12

3. Data: FNAME(5)
   Format: A12

4. Data: FNAME(6)
   Format: A12

5. Data: FNAME(4)
   Format: A12

6. Data: FNAME(7)
   Format: A12

7. Data: FNAME(8)
   Format: A12

An example of INFILE.MOD is given below:

```
                                          Input Records
Data                     Explanation    |---+----+----+----+
item                                    1   5   10   15   20
 1.      FNAME(12)----------------------MODAIR.PRN
 2.      FNAME(3)-----------------------BASAIR4.PRN
 3.      FNAME(5)-----------------------BCFAIR4.PRN
 4.      FNAME(6)-----------------------SIPAIR4.PRN
 5.      FNAME(4)-----------------------OCAIR4.PRN
 6.      FNAME(7)-----------------------HEAD4.BIN
 7.      FNAME(8)-----------------------FLOW4.BIN
```

See Section 3.3.3 for a definition of variables included in INFILE.MOD.

3.3.10 PREAIR Model Information Output File MODEL.DAT

The preprocessor outputs information on model units, physical parameters, cell-layer depths and well/trench locations, and pressures directly to the file MODEL.DAT, which is subsequently read by POSTAIR. This process provides a mechanism for transferring selected data between the preprocessor and the postprocessor. For cases in which the postprocessor is used independently of the preprocessor, the user must create the MODEL.DAT file manually. The name MODEL.DAT is specified in both the pre- and postprocessor input files. The file name must remain constant throughout a particular AIR3D simulation.

The file MODEL.DAT consists of several lines. The first line consists of the unit system being used in the model as well as the number of wells and trenches in the model. The second line consists of three entries--namely, the ground-surface elevation, the thickness of the superimposed atmospheric layer, and the air temperature. Each of the next NLAY lines in MODEL.DAT consists of a single entry that represents the depth from the ground-surface elevation to the bottom of consecutive cell layers. The final data lines in MODEL.DAT comprise data on well and trench configurations and pressures. Units used in the MODEL.DAT file must correspond to the unit system selected to enter data into PREAIR in the file DATAIRx.PRE. The postprocessor makes the necessary conversions according to the selections made in the first line of

MODEL.DAT. Well and trench data are used in the mass-balance computations. Layer-depth data from MODEL.DAT are used to calculate the vertical coordinates of the output parameters. The postprocessor uses the temperature data from MODEL.DAT to correct the viscosity term in the air-flow rates. The information contained in the MODEL.DAT file must be present to implement POSTAIR.

MODELx.DAT file specifications are as follows:

Name of file:	Specified by user in file INFILEx.PRN (for example, MODEL4.DAT)
File contents:	Unit system; number of wells; number of trenches; ground surface elevation; thickness of superimposed atmospheric layer; air temperature; depth from ground surface to bottom of consecutive cell layers; well start and end row, column, and layer; well pressure, trench start and end row, column, and layer; and trench pressure.
File application:	This preprocessor output file is used to transfer selected model data from the preprocessor to the postprocessor.
Fortran unit number:	The program defines the output file as UNIT = 19.
Program output:	Output is controlled in the subroutines SETUP and MODBCF. Output is written directly to the file.
Physical units:	Unit systems for temperature and length should correspond to the original unit system used in the DATAIRx.PRE input file. If no unit system is specified, units must conform to the default unit systems for each parameter.

The structure of MODELx.DAT is as follows:

1. Data: IU1(1),IU1(2),IU1(3),IU1(4),IU1(5),IU1(6),IU1(7),NWELL,NTRCH
   Format: 9I5

2. Data: GELEV,BSURF,TAIR
   Format: 3F10.2

Input item 3 NLAY times (once for each cell layer).

3. Data: ZDEPTH
   Format: F10.2

If NWELL > 0 then input item 4 IW=1,2,..,NWELL times (once for each well), otherwise omit.

4. Data: IWELL(IW,1),IWELL(IW,2),IWELL(IW,3),IWELL(IW,4),IWELL(IW,5), IWELL(IW,6),IWELL(IW,7),SHW(IW)

   Format: 7I5,E20.8

IF NTRCH > 0 then input item 5 IT=1,2,..,NTRCH times (once for each trench), otherwise omit.

5. Data: ITRCH(IT,1),ITRCH(IT,2),ITRCH(IT,3),ITRCH(IT,4),ITRCH(IT,5), ITRCH(IT,6),ITRCH(IT,7),TSHD(IT)

   Format: 7I5,E20.8

An example of MODELx.DAT is given below:

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

1.     IU1(1),...,IU1(7),NWELL,NTRCH——        1    1    1    1    1    1    1    1    0
2.     GELEV,BSURF,TAIR————————                 0.00      20.00      10.00
3a.    ZDEPTH——————(layer 1)——              100.00
3b.    ZDEPTH——————(layer 2)——              200.00
3c.    ZDEPTH——————(layer 3)——              300.00
4.     IWELL(I,1),...,IWELL(I,7)————        1    3    3    4    4    3    3         .90000000E+00
```

The definitions of the variables included in the output file MODEL.DAT are presented below. Variables are presented in the order in which they appear in the data file. Variable units must be consistent with the units used to enter data into the preprocessor. Information on variables not discussed below can be found in Section 3.3.4.

GELEV

- GELEV is a reference datum used for obtaining elevations in model layers. The input value should correspond with the elevation of the ground surface. (Note that this value will not coincide with that for the uppermost model layer because the preprocessor superimposes an additional cell layer on the geologic domain. The postprocessor uses GELEV to calculate elevations at various points in the model domain (at centers of layers, layer interfaces, and so on). Depending on the selection of GELEV, the elevations can be negative or positive. For example, if GELEV is specified as 0.0 cm and the layer thickness is 100 cm, then the elevation at the bottom of the first layer will be -100.0 cm. Alternatively, for GELEV equal to 1,000.0 cm, the elevation at the bottom of the first layer will be 900.0 cm. When PREAIR is used to set up the model simulation, GELEV is specified automatically.

- GELEV defaults to a value of 0.0 if the user does not specify a value. Note that for GELEV = 0.0 the elevation of model layers will be negative. If GELEV is sufficiently large, then the elevation of the model layers will be positive.

BSURF

- BSURF is the thickness in the Z-direction of the cell layer superimposed on the model domain to satisfy the atmospheric-recharge boundary conditions. BSURF is used to generate vertical or Z-coordinates for air-flow rates from the atmosphere. When PREAIR is used, BSURF is specified automatically.
- BSURF must be present in MODEL.DAT for all air-flow simulations.

TAIR

- TAIR is the temperature of the air during the simulation. TAIR is used to correct the air viscosity for temperature. The corrected air viscosity is then used in both the volumetric and mass air-flow-rate calculations. When PREAIR is used to set up the model simulation, TAIR is set up automatically. TAIR is not defined in the MODFLOW documentation.
- TAIR defaults to a value of 283.15 K if not specified by the user.

ZDEPTH

- ZDEPTH is the depth to the bottom of consecutive cell layers from the ground-surface elevation (GELEV). One value must be input per line for each cell layer specified by the user. The values are used in the postprocessor to calculate the vertical coordinates of various output parameters in each cell layer. When PREAIR is used, ZDEPTH is specified automatically.
- ZDEPTH must be specified for each cell layer in order to implement the air-flow postprocessor. Input must always be positive.

3.3.11 PREAIR Input File INFILEx.POS

The preprocessor creates an input file for direct use with the postprocessor. The file INFILEx.POS contains default values for simulation output, names of files containing MODFLOW data, and the name of a file containing selected model information. The postprocessor can be used to enter INFILEx.POS directly, modify the contents of INFILEx.POS, or create a new INFILEx.POS file according to user needs. The contents of INFILEx.POS are discussed in detail in Section 4.5.3.

SECTION 4.0--POSTAIR POSTPROCESSOR TO MANAGE OUTPUT FROM MODFLOW FOR AIR-FLOW SIMULATIONS

The postprocessor POSTAIR is a Fortran code that accesses binary files generated by MODFLOW for analysis and graphical presentation. POSTAIR can be used to organize output for both air-flow and ground-water-flow simulations. Note that this manual deals only with air-flow applications.

4.1 POSTAIR Applications

For air-flow simulations, POSTAIR can be used to transform output into dimensionally consistent air-flow parameters (see Section 2.3), and to organize output according to user specifications. The transformations available in POSTAIR for generating pneumatic parameters are as follows:

- pressure in the model cells, from head output
- volumetric flow rates at constant-head cells and through active cell faces, from head and flow output
- mass flow rates at constant-head cells and through active cell faces, from flow output
- flow to/from wells and trenches from head and flow output
- mass flow balances for air entering and leaving the domain.

POSTAIR can be used to organize output according to the following categories:

- type of output (pressure and (or) flow--Section 4.3.3)
- orientation of output (layer, row, or column--Section 4.3.4)
- format of output (single or multiple files, text or binary files-- Section 4.3.5)
- extent of output (partial or complete listings of output data-- Section 4.3.6)
- nature of output (vector components or resultants--Section 4.3.7).

The postprocessor writes to separate files the output data for two-dimensional sections in the model domain. Postprocessor output is written in accordance with the parameter type and sort criteria specified by the user. Output-file names are generated by the postprocessor according to the convention described in Section 4.4. Typical information contained in the output files includes the following:

- spatial coordinates for each of the directions in the specified plane
- parameter values
- nodal coordinates for each of the directions in the specified plane.

MODFLOW uses the assumption that the origin of the spatial and nodal coordinates is located in the rear upper-left-hand corner of the model domain. This convention is appropriate for plotting two-dimensional vertical (X-Z or Y-Z) slices through the model domain. When generating two-dimensional representations of the horizontal (X-Y) plane, however, the MODFLOW convention can result in inverted graphical output, as many graphics packages require that the origin of the coordinate systems be in the lower left-hand corner of the two-dimensional slice. The postprocessor provides the option of defining the coordinate systems (see Section 4.3.1) as follows:

- use the MODFLOW convention
- for horizontal slices, redefine the MODFLOW spatial-coordinate origin to coincide with the lower left-hand corner of the two-dimensional section but retain the original nodal configuration
- for horizontal slices, redefine both the MODFLOW spatial and nodal coordinate origins to coincide with the lower left-hand corner of the two-dimensional slice.

In air-flow simulations, the preprocessor superimposes an additional model layer on the geologic domain set up by the user. The postprocessor recognizes this addition and corrects the model output to conform with the original layer numbering (the superimposed layer, when referenced, is assigned a layer number of zero).

Total net flow rates at the centers of constant-head cells are calculated by MODFLOW. Components of the flow rates at the faces of active cells also are computed by MODFLOW. The postprocessor assigns to flow rates either two- or three-dimensional coordinates that represent their points of application. In the case of active cells, the user has the option of selecting coordinate output that corresponds to either the cell faces or the cell centers. Although the exact point of application of flow components through active cells is at the cell faces, the geometric displacement to the cell centers can be a useful approximation when plotting flow vectors for two-dimensional sections that show flow paths in the model domain.

The following sections describe the transformations necessary to generate air-flow output, options available for organizing model output and input, and output data requirements.

4.1.1 Pneumatic Pressure Transformation

As described in Section 2.3.1, head output directly from MODFLOW for pneumatic simulations corresponds to air pressure squared, with units of $(g/cm\text{-}s^2)^2$. Hence, the transformation performed by the postprocessor to obtain the pneumatic equivalent of head is as follows:

$$P = \frac{H_{MOD}^{1/2}}{C} \qquad (23)$$

where

P	=	Air Pressure at cell center	[atm]
H_{MOD}	=	MODFLOW head output value	$[g/cm\text{-}s^2]^2$
C	=	factor to Convert Units = 1,013,250	$[g/cm\text{-}s^2\text{-}atm]$

4.1.2 Pneumatic Volumetric Flow Rate Transformation

As described in Section 2.3.2, flow values that are output directly from MODFLOW for pneumatic simulations correspond to a term with units of g^2-cm/s^4. Hence, the transformation performed by the postprocessor to obtain the volumetric air-flow rate is as follows:

$$F_{vol} = \frac{F_{MOD}}{2\,\mu\,H_{MOD}^{1/2}} \qquad (24)$$

where

F_{vol}	= volumetric air flow	[cm^3/s]
F_{MOD}	= MODFLOW flow output value	[g^2-cm/s^4]
μ	= dynamic air viscosity	[g/cm-s]

4.1.3 Pneumatic Mass Flow Rate Transformation

As described in Section 2.3.2, flow values that are output directly from MODFLOW for pneumatic simulations correspond to a term with units of g^2-cm/s^4. The transformation performed by the postprocessor to obtain the mass air-flow rate is as follows:

$$F_{mass} = \frac{\omega\,F_{MOD}}{2\,\mu\,R\,T} \qquad (25)$$

where

F_{mass}	= mass air flow	[g/s]
ω	= average molecular weight of air	[g/mol]
μ	= dynamic viscosity of air phase	[g/cm-s]
R	= universal gas constant	[g-cm^2/s^2-mol-K]
T	= temperature	[K]

4.1.4 Spatial Coordinates for Pressure and Flow Output

MODFLOW generates both head and flow output. The postprocessor assigns spatial coordinates that identify the point of application of the particular output variable. Coordinates in the horizontal (X-Y) plane are calculated from cell widths defined in the MODFLOW Block-Centered-Flow file. Coordinates in the vertical (Z)-direction are calculated from information contained in the data file MODEL.DAT. For air-flow simulations, MODEL.DAT is generated directly by the preprocessor PREAIR. For ground-water simulations, MODEL.DAT must be created by the user. Requirements for MODEL.DAT are discussed in Section 3.3.10.

Pressure values in air-flow simulations are generated at the center of each cell in the model domain. Hence, the spatial coordinates determined by the postprocessor represent the coordinate values at the centers of respective model cells.

Air-flow components are generated by MODFLOW for each cell in the model domain as follows:

- For net flow rate at a constant-head cell, the spatial coordinates correspond to the center of the cell.
- For the X-component of flow, the spatial coordinates correspond to the center of the right face of the cell.
- For the Y-component of flow, the spatial coordinates correspond to the center of the front face of the cells.
- For the Z-component of flow, the spatial coordinates correspond to the center of the lower face of the cells.

Spatial coordinates are output whenever pressure or flow parameters are written to data files by the postprocessor. POSTAIR provides several options to vary the coordinate output to correspond with the users graphical environment as follows:

- coordinates for flow components at faces can be changed to coordinates at cell centers (Section 4.3.1)
- coordinate origins in horizontal sections can be relocated (Section 4.3.2)
- two- or three-dimensional spatial coordinates can be generated (Section 4.3.6).

4.1.5 POSTAIR Settings and Units Used in Air-flow Simulations

The universal gas constant (R) and average molecular weight of air (ω) are defined within the postprocessor. The temperature of the air (T) can be either specified by the user (in the MODEL.DAT file) or defaulted to a value of 10° C. The value of the air-phase viscosity (μ) is calculated within the program and depends on the temperature of the air (see Section 3.1.7). The postprocessor defines the following variables internally:

· $R = 8.314 \times 10^7$	[g-cm^2/s^2-mol-K]
· $\omega = 28.8$	[g/mol]
· T = 283.15 (or user input value)	[K]
· $\mu = 1.76 \times 10^{-4}$ (reference at 10°C)	[g/cm-s]
· 1 atmosphere = 1,013,200	[g/cm-s^2]

The above values have been specified in the code PREAIR. If changes are necessary, the user must incorporate them within PREAIR.

4.1.6 POSTAIR Units

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

- length units, where
  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

- volume units, where
  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

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

- pressure units, where
  1 atm = 760 mm of Hg = 406.794 in. H_2O = 101.325 kPa = 14.696 lb/in^2

- temperature units, where
  tc °C = tk - 273.15 K = (tf - 32) / 1.8 °F

- mass units, where
  1 g = 1.0 x 10-3 kg = 2.2046 x 10-3 lb

- permeability units, where
  1 cm2 = 1.0 x 10-2 dm2 = 1.0 x 10-4 m2 = 1.550 x 10-1 in2
  = 1.076 x 10-3 ft2 = 1.1962 x 10-4 yd2 = 1.0 x 108 darcy

The user can select any combination of the above unit systems provided that all data are entered in the selected system. If no unit system is specified, PREAIR defaults to the first unit system in the listings above.

4.2 POSTAIR System Configuration

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

4.2.1 Mainframe or Personal Computers

For operation on a mainframe computer, the following section of code in the main calling program appears as follows:

```
C
C4----ASSIGN INPUT UNIT AND PRINTER UNIT
C
C      SET  :  IV(81) = INBAS = 5 WHEN USING IBM PC OR MAC
C      SET  :  IV(81) = INBAS = 1 WHEN USING MAIN FRAME
C
C      SET  :  IV(82) = IOUT  = 6 WHEN USING IBM PC OR MAC
C      SET  :  IV(82) = IOUT  = 1 WHEN USING MAIN FRAME
C
       INBAS = 1
       IOUT  = 1
```

For operation on a personal computer, the following section of code in the main calling program appears as follows:

```
C
C4----ASSIGN INPUT UNIT AND PRINTER UNIT
C
C      SET  :  IV(81) = INBAS = 5 WHEN USING IBM PC OR MAC
C      SET  :  IV(81) = INBAS = 1 WHEN USING MAIN FRAME
C
C      SET  :  IV(82) = IOUT  = 6 WHEN USING IBM PC OR MAC
C      SET  :  IV(82) = IOUT  = 1 WHEN USING MAIN FRAME
C
       INBAS = 5
       IOUT  = 6
```

4.2.2 Array Dimensions

Memory allocation for storage of real and integer variables in the air- flow postprocessor is specified by using the arrays XX(LENX) and IX(LENI), respectively. The sizes of the arrays are specified by using a PARAMETER statement in the main program. For program applications on a mainframe or personal computer, the array size can be redefined to meet the system capacity. The postprocessor performs a check to determine whether the model storage requirements are adequate for the proposed application. If the allocated storage requirements are exceeded, the user must redimension the arrays by increasing the values of LENX or LENI in the PARAMETER statement in the main code. The following section of code from the subroutine SETUP shows the storage-space check performed and the accompanying output message.

```
C
C-----TEST MEMORY ALLOCATION AREA FOR IX ARRAY
C
      IIEND=IEND1
      IF(IIEND.LT.IEND2) IIEND=IEND2
      IF(IIEND.GT.IV(84)) THEN
       WRITE(IOUT,441)IIEND+100
       WRITE(IOUT,442)
       STOP
      END IF
 441  FORMAT(///////,T10,'REDIMENSION IX ARRAY TO LENI = ',I10)
 442  FORMAT(//,T10,'OR REDUCE NCOL, NROW, NLAY IN INPUT DATA')
C
C-----TEST MEMORY ALLOCATION AREA FOR XX ARRAY
C
      IXEND=IXEND1
      IF(IXEND.LT.IXEND2) IXEND=IXEND2
      IF(IXEND.GT.IV(83)) THEN
      WRITE(IOUT,445)IXEND+100
      WRITE(IOUT,446)
       STOP
      END IF
 445  FORMAT(///////,T10,'REDIMENSION XX ARRAY TO LENX = ',I10)
 446  FORMAT(//,T10,'OR REDUCE NCOL, NROW, NLAY IN INPUT DATA')
```

If the message of statements 441 and 442, or, 445 and 446 above appears during operation of the postprocessor, the values of LENX and LENI need to be changed in the main program by modifying the PARAMETER statement below:

```
C
C3----SPECIFICATIONS:
C
      PARAMETER(LENX=1000000,LENI=100000)
      COMMON XX(LENX),IX(LENI),AX(50)
```

4.2.3 Compilation and Execution of POSTAIR on a Mainframe or Personal Computer

Whenever modifications or changes are made to the postprocessor source code, the program must be recompiled so that the alterations are incorporated in 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. The preprocessor PREAIR, the postprocessor POSTAIR, and MODFLOW codes must be compiled by using the same compiler; otherwise, inconsistencies in transferring binary output between programs can be encountered. The following lines comprise a CPL file to compile and execute the air-flow postprocessor on a PRIME mainframe computer. Adjustments to the commands below probably will be necessary to operate the programs on your system.

```
F77 POSTAIR.F77
&DATA SEG -LOAD
LOAD POSTAIR
LI
SA
QU
&END
SEG POSTAIR
```

The following commands were used to compile and link the postprocessor on an IBM personal computer with Microsoft's Fortran compiler:

```
FL POSTAIR.FOR
```

To execute the postprocessor on a personal computer, make current the directory containing the executable code (for example, POSTAIR.EXE, created in the above compilation step) and at the prompt enter:

```
POSTAIR
```

On both mainframe and personal computers, the introductory screen shown below appears prompting the user to select a particular option.

```
POSTAIR - AN AIR-FLOW POSTPROCESSOR (Ver 1.1)
======== === ========= =============== ======

DEVELOPED BY :  CRAIG J. JOSS

                ARTHUR L. BAEHR

 SELECT :

1. TO RUN POSTAIR USING AN EXISTING INPUT FILE

2. TO MODIFY AN EXISTING INPUT FILE

3. TO CREATE A NEW DATA INPUT FILE

4. TO EXIT POSTAIR


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

In order to use Option 1 and Option 2, the data file INFILEx.POS (Section 4.5.3) must exist. Upon entering 1 or 2, the user is prompted for the name of the INFILEx.POS file. For Option 1, the simulation then transforms and organizes the MODFLOW output files. For Option 2, the contents of INFILEx.POS are displayed on the screen in sequence. The user can then change the data by entering a new value or retain the existing data by simply pressing the ENTER or CARRIAGE RETURN key. After the user makes the changes, POSTAIR saves the modified INFILEx.POS file and returns the user to the main menu. The user can then proceed with the simulation by selecting Option 1.

Option 3 can be used to set up data in the file INFILEx.POS. After setting up INFILEx.POS by selecting Option 3, the program returns to the above menu, where the user can proceed with the simulation (Option 1), make additional changes to INFILEx.POS (Option 2), or exit POSTAIR (Option 4).

Option 4 is used to exit the program. After successful application of the postprocessor, a message is displayed that describes the names of the files that were set up. The display below shows a typical output message generated by the postprocessor.

```
POSTAIR - AN AIR-FLOW POSTPROCESSOR (Ver 1.1)
======= === ======== ============= =====


POSTAIR has generated PRESSURE text files              : APxxxx.Txx

POSTAIR has generated VOLUMETRIC text files            : AVxxxx.Txx

POSTAIR has generated MASS text files                  : APxxxx.Txx

POSTAIR has generated MASS BALANCE / WELL text files   : APxxxx.Txx
```

A detailed description of output-file names is given in Section 4.4. Depending on the user settings, output is written to either text files (with extensions xxx.Txx) or binary files (with extensions xxx.Bxx).

4.3 <u>POSTAIR Options for Organizing MODFLOW Output</u>

A given graphics software package can require a different origin definition than that used by MODFLOW. This section describes the options available for redefining the output origin.

4.3.1 Options for Relocating Coordinate Origins

When defining the model domain in MODFLOW, the presence of a spatial coordinate system and a nodal coordinate system must be recognized. The spatial coordinate system defines the distances of consecutive cells from a given origin. The nodal coordinate system defines row, column, and layer indices. Separate spatial and nodal coordinates apply to cells along each of the three orthogonal axes (X, Y, and Z). Hence, depending on the location of the origin, significantly different outputs can be obtained for the coordinate systems in each of the principal directions. A MODFLOW model comprises a three-dimensional domain in which the origin of each coordinate system is located at the top rear left-hand corner of the domain, as indicated below:

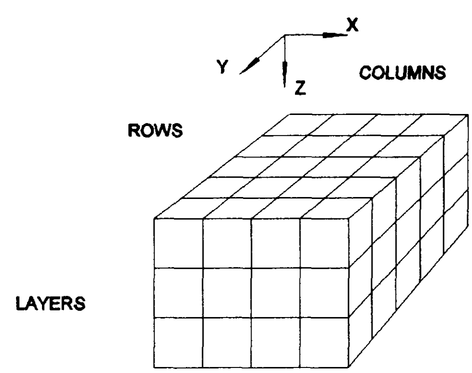

Figure 2.--Three-dimensional MODFLOW coordinate origins.

Sections through the three-dimensional MODFLOW domain are two-dimensional slices in the X-Y, X-Z,and Y-Z planes, respectively. According to the convention used in MODFLOW, the origins of the spatial and nodal coordinates of these two-dimensional slices are located at the upper left-hand corner of a slice, as indicated in Figure 3.

By relocating the position of either the spatial or the nodal origin, it is possible to generate equivalent, but transformed, coordinate output. The postprocessor provides three options for locating the spatial and nodal origins:

(1) Spatial and nodal origins can be located in the upper left-hand corner (MODFLOW convention).
(2) The nodal origin can be located in the upper left-hand corner (MODFLOW convention) but the spatial origin is relocated to the lower left-hand corner.
(3) Spatial and nodal origins both can be relocated to the lower left- hand corner.

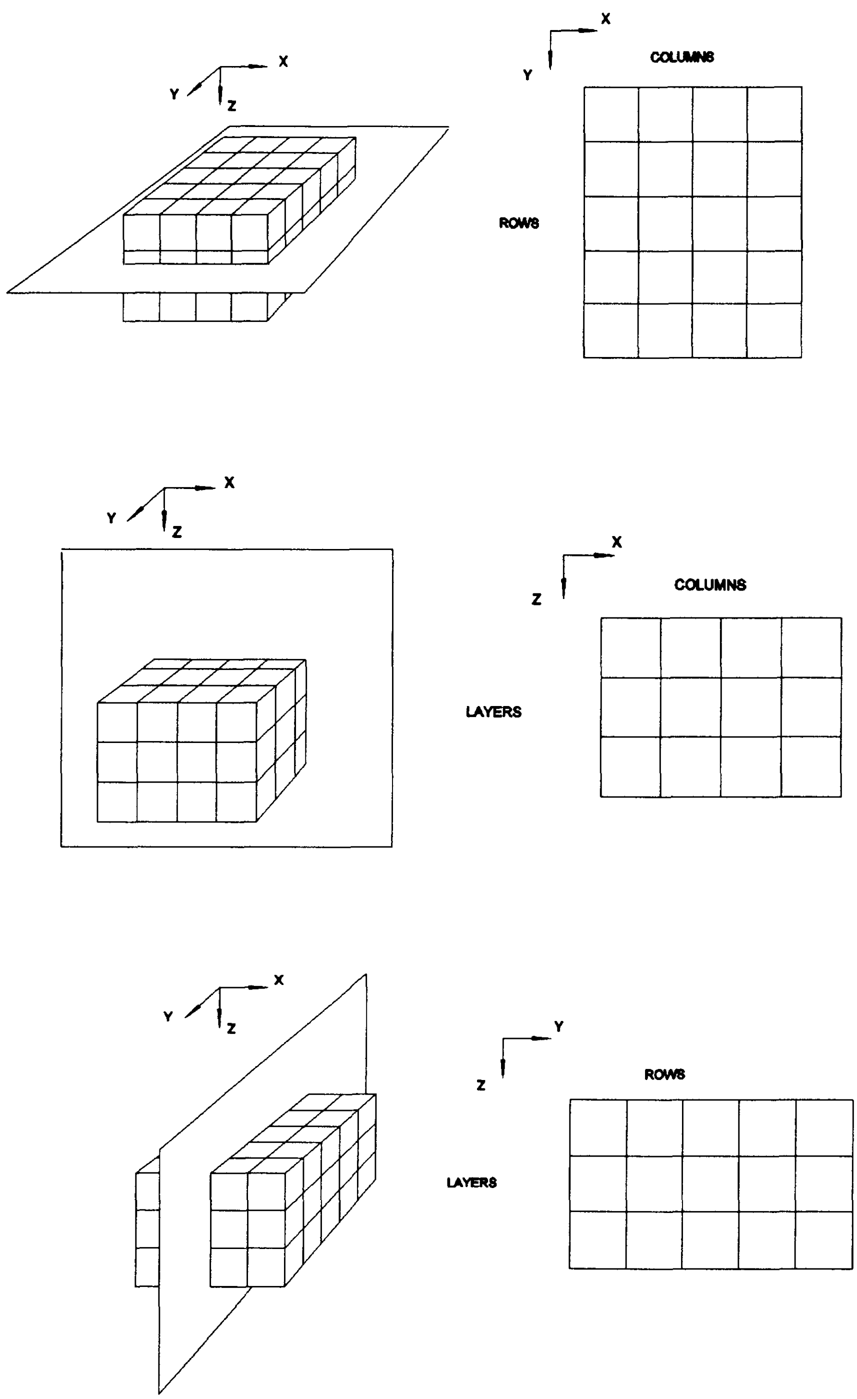

Figure 3.--Two-dimensional MODFLOW coordinate origins.

The options apply only to the output of spatial and nodal coordinate values in two-dimensional slices through the model. Depending on the orientation of the two-dimensional slices, the following restrictions apply:

- Output by layer (horizontal slices in X-Y plane) allows option 1, 2, or 3 to be specified.
- Output by row (vertical slices in X-Z plane) allows only option 1 to be specified.
- Output by column (vertical slices in Y-Z plane) allows only option 1 to be specified.

To obtain output by layer, transformation of the coordinate origins by selecting option 2 or 3 is necessary to ensure consistency with graphical packages in which origins are located in the lower left-hand corner. For output by rows or columns, transformation of coordinate origins with option 2 or 3 would result in an inversion of the model domain; that is, the ground-water boundary would appear at the top of the section and the atmospheric boundary would appear at the bottom. Therefore, if these options are accidentally selected, the postprocessor reassigns option 1.

In summary, option 1 in the postprocessor specifies the spatial and nodal coordinate origins as shown in figure 4.

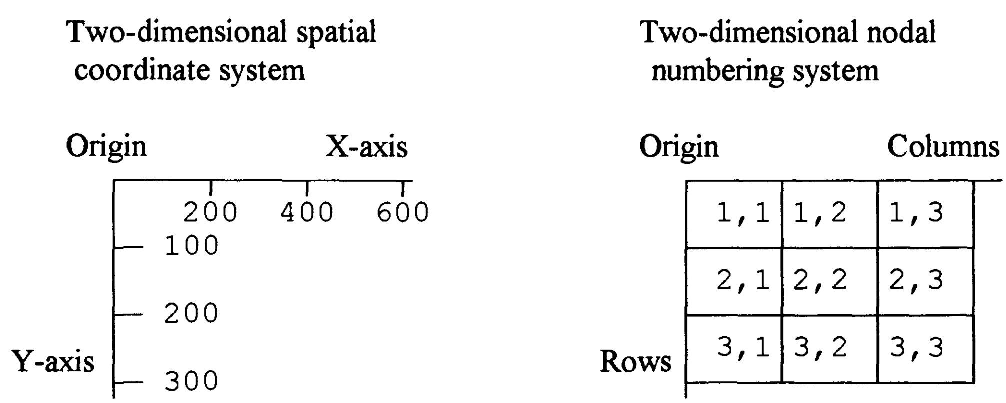

Figure 4.--Output coordinate system for option 1.

The transformation resulting from selecting option 2 is shown in figure 5.

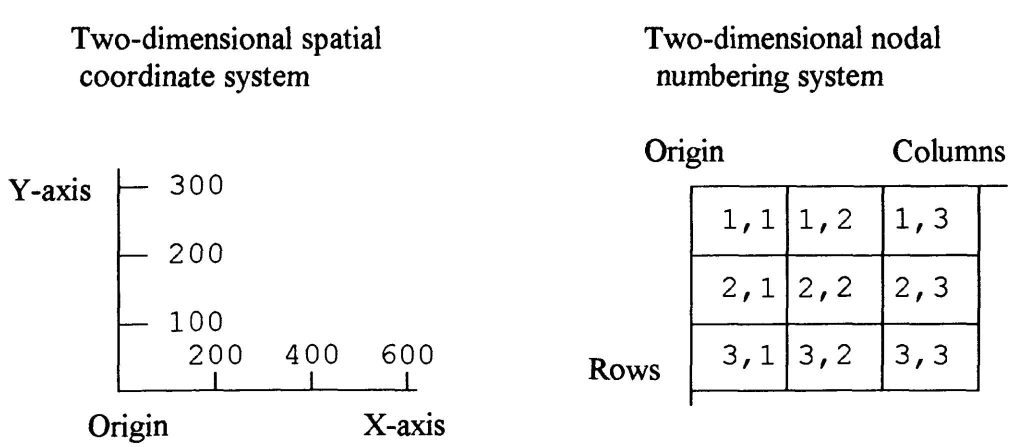

Figure 5.--Output coordinate system for option 2.

The transformation resulting from selecting option 3 is shown in figure 6.

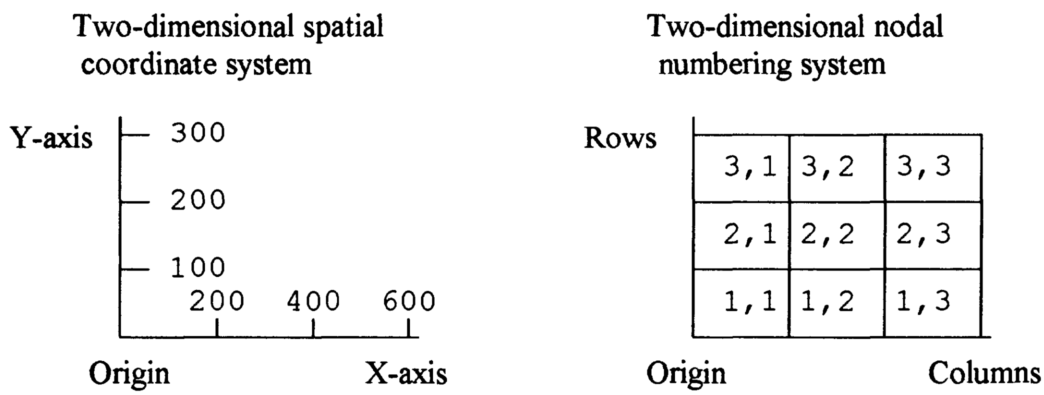

Figure 6.--Output coordinate system for option 3.

4.3.2 Options for Spatial Coordinate Locations for MODFLOW Output

The postprocessor reads and transforms MODFLOW output, and assigns to it either two- or three-dimensional spatial coordinates. Coordinates assigned to the pressure output represent cell centers. No options exist for varying the coordinate locations of pressure output. The spatial coordinates assigned to the flow output depend on the particular flow value being calculated. MODFLOW generates four types of flow output, as follows:

- net flow at constant-head cells (Fc)
- flow component in the X-direction at active cells (F_x)
- flow component in the Y-direction at active cells (F_y)
- flow component in the Z-direction at active cells (F_z).

In the case of constant-head cells, coordinates assigned to F_c represent the cell centers. No options exist for varying the coordinate locations of F_c. In the case of active cells, coordinates assigned to the flow components represent the cell faces. The flow component F_x is applied at the center of the right face of the model cell, F_y is applied at the center of the front face, and F_z is applied at the center of the lower face. The points of application of the calculated flow rates are shown in figure 7.

In certain instances, such as when component flow rates are plotted, it may be desirable to approximate the points at which these flow rates act by displacing the points of application from the cell faces to the centers of the model cells. The postprocessor provides the option of performing this displacement. However, it does not adjust the output values of F_c, F_x, F_y, and F_z to conform with the new spatial coordinates. The points of application of the shifted flow rates are shown in figure 8.

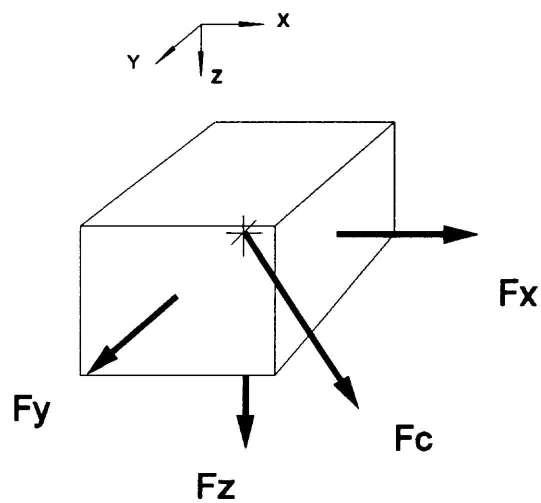

Figure 7.-- Flow rates at cell faces.

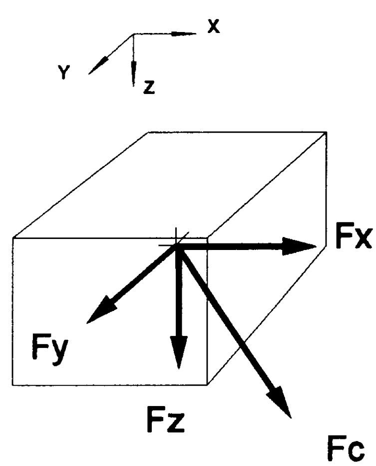

Figure 8.--Flow rates at cell centers.

4.3.3 Options For Specifying Type of Output

For air-flow simulations, the postprocessor first transforms the MODFLOW output, and then provides options to generate output by either of the following groups of pneumatic parameters:

- pressure in the model cells (generated from head output)
- pressure, and volumetric and mass flow rates (generated from head and flow output).

Because pressure values are required to compute volumetric flow, no option is provided to output flow without pressure. The user also has the flexibility to select or screen particular data sets.

4.3.4 Options For Specifying Orientation of Output

Each of the output types can then be sorted by geometric orientation, as follows:

- output sorted by layer (horizontal, X-Y slices)
- output sorted by row (vertical, X-Z slices)
- output sorted by column (vertical, Y-Z slices).

An exception to sorting output by the above categories arises when pressure and flow predictions are written in a single file format (see Section 4.3.5). In such cases, output can be oriented only by layers. When the simulation results are written in the separate file format, however, all of the above options apply. In such cases, each output item in consecutive layers, rows, or columns is written to a separate file. File names are generated internally by the postprocessor according to the convention described in Section 4.4.

4.3.5 Options For Specifying Format of Output

In specifying the format of output, the user can

(1) generate single files--one for pressure, one for volumetric flow, and one for mass flow output at specified two-dimensional slices;
(2) generate separate files for each pressure and flow component (nine parameters) at specified two-dimensional slices;
(3) generate separate files for each pressure, flow component, and two-dimensional flow resultants at specified two-dimensional slices;
(4) generate separate files for each pressure and flow component at specified two-dimensional slices, and output three-dimensional flow resultants at each cell location.

If option (1) is selected the output can be written in either a text or a binary format. If option 2, 3 or 4 is selected the output can be written only in a text format. If option 1 is selected, three files are generated, as follows:

- a file containing pressure data at a single slice or at every two-dimensional slice sorted by layers;
- a file containing volumetric flow components at a single slice or at every two-dimensional slice sorted by layers;
- a file containing mass flow components at a single slice or at every two-dimensional slice sorted by layers.

In text output associated with option 1, the pressures and flows are defined by using three spatial coordinates and three nodal coordinates. In binary output associated with option 1, the files resemble MODFLOW head and flow binary output, which consists solely of parameter values (that is, no coordinates are included in the binary files). If option 2 is selected, pressure and flow components are written to separate files, depending on the slices specified, which include

- NN files with pressure output
- NN files with net volumetric flow at constant-head cells
- NN files with X-component of volumetric flow at active cells
- NN files with Y-component of volumetric flow at active cells
- NN files with Z-component of volumetric flow at active cells
- NN files with net mass flow at constant-head cells
- NN files with X-component of mass flow at active cells
- NN files with Y-component of mass flow at active cells
- NN files with Z-component of mass flow at active cells

where NN = number of rows, columns, or layers (or NN = 1 for a single slice) depending on the orientation of the output. If option 2 is selected, only text output can be generated. The pressures and flows in option 2 are defined by two spatial coordinates and two nodal coordinates. Option 3 output encompasses all of option 2 output at the specified slices as well as combinations of two-dimensional flow components. Only text output can be generated if option 3 is selected. Option 4 output encompasses all of option 2 output at the specified slices, as well as combinations of three-dimensional flow components at each cell location. Only text output can be generated if option 4 is selected.

4.3.6 Options For Specifying the Extent of Output

The extent of the output depends largely on the two-dimensional slices specified by the user. POSTAIR currently offers two choices for specifying slices to be written to output files. The first choice is to specify a particular layer, row, or column. In this case, only pressure and flow data corresponding to the specified slice are written to the output files. The second choice specifies that pressure and flow data for every layer, row, or column be written to the output files. The user selection, then, significantly affects the postprocessor execution times and memory storage requirements.

If output for a particular slice is specified, the number of files generated will be nine--one pressure file, four volumetric flow files, and four mass flow files. If output at every two-dimensional slice is specified, the resulting number of files will be nine times the number of rows, nine times the number of columns, or nine times the number of layers. If, in addition, two-dimensional resultant flow output is selected, additional files (two for the single-slice case, or two times the number of rows, two times the number of columns, or two times the number of layers for the multiple-slice case) will be generated. Similarly, if three-dimensional resultant flow output is selected, additional files (one for mass-flow and one for volumetric-flow resultants at each cell location) will be generated.

4.3.7 Options For Specifying the Nature of Output

Pressure output consists of scalar values assigned to cell centers in the model domain. Flow output assigned to active cells has three orthogonal components through the cell faces. The postprocessor provides options for combining either two or three orthogonal flow components to generate flow resultants. When two flow components are combined, the magnitudes and directions of the resultant flows lying in the two-dimensional slice being investigated are output and may be used directly in certain graphical packages. When all three flow components are combined, only the magnitudes of the three-dimensional resultant flows at each cell in the domain are output.

In combining the flow components, the postprocessor follows the MODFLOW convention, namely, that:

- flow components are positive in the X-direction from left to right
- flow components are positive in the Y-direction from rear to front
- flow components are positive in the Z-direction from top to bottom.

The two-dimensional resultant flows are generated by averaging flow into and out of the cell in a particular direction. Two averaged flow values, in orthogonal directions, are then combined to obtain the magnitude and direction of the resultant. Two values of the flow resultants are reported, one using averaged flows through the entire cell face and the other using averaged flows per unit area through the cell face. The procedure is illustrated with an example below.

Consider flow output from a pneumatic simulation sorted by layers. The postprocessor uses flow components from the X- and Y-directions to perform the calculations. The procedure outlined below is applied to both volumetric and mass flows. Output from each type of flow is written to separate files; one file is generated for each two-dimensional slice oriented according to the user specifications. Note that, as described in Section 4.3.6, it is also possible to select output so that resultant flows are generated only for a single slice. Further, output file names are generated directly by the postprocessor according to the convention discussed in Section 4.4.

Resultant two-dimensional flows through cell faces at interior cells are calculated as follows:

In the X-direction (along rows):

$$F_{Xave} = \frac{F_{X1} + F_{X2}}{2} \qquad (26)$$

where

F_{Xave} = X flow component assigned to cell
F_{X1} = flow component into cell (at left face) in X-direction
F_{X2} = flow component out of cell (at right face) in X-direction.

In the Y-direction (along columns):

$$F_{Yave} = \frac{F_{Y1} + F_{Y2}}{2} \qquad (27)$$

where

F_{Yave} = Y flow component assigned to cell
F_{Y1} = flow component into cell (at rear face) in Y-direction
F_{Y2} = Flow Component out of Cell (at front face) in Y-direction.

Resultant two-dimensional flows through the cell face $F_{X\text{-}Y}$ in the X-Y slice:

$$F_{X\text{-}Y} = [(F_{Xave})^2 + (F_{Yave})^2]^{1/2} \qquad (28)$$

Direction of resultant two-dimensional flow in the X-Y slice:

$$\text{Angle(X-Y)} = \arctan \left(\frac{F_{Yave}}{F_{Xave}}\right) \qquad (29)$$

where

Angle(X-Y) = angle of resultant flow vector relative to the X- or horizontal axis [degrees]

Note that for boundary cells, where the only flow present is the flow out of the cell (atmospheric recharge), the postprocessor assigns this value to the average flow rate. For resultant two-dimensional flows per unit area through the cell face, F_{Xave} and F_{Yave} are replaced in the above procedures with (F_{Xave}/A_x) and (F_{Yave}/A_y), respectively, where A_x is the area of the cell face in the X-direction and A_y is the area of the cell face in the Y-direction.

Two-dimensional plots of flows provide a means to rapidly visualize flow paths and the effects of various boundary conditions and stratigraphy on flow in the model domain. The input requirements to graphical packages used to plot the two-dimensional resultants vary. Some packages require that two-dimensional vectors be input in terms of magnitude and direction. In such cases, the option to generate the flow-rate resultants with the postprocessor would be selected; however, graphical packages also are available that allow the vectors to be input in terms of their X- and Y-components. In these instances, the output files containing flow rates through the cell faces would be used directly. This procedure reduces the postprocessor computing time and disk storage requirements. When orthogonal flow-rate values are used directly, the sign convention of the graphical package must be compatible with that used by MODFLOW. In particular, MODFLOW assumes that downward vertical flow components are positive, whereas other packages assign positive values to upward vertical vectors.

Resultant three-dimensional flows at cells in the model domain are calculated as follows:

In the X-direction (along rows):

$$F_X = \frac{F_{X1}}{A_X} \tag{30}$$

where

F_X = X flow component per unit area assigned to cell,
F_{X1} = flow component out of cell (at right face) in X-direction,
A_X = area of cell (at right face) in X-direction.

In the Y-direction (along columns):

$$F_Y = \frac{F_{Y1}}{A_Y} \tag{31}$$

where

F_Y = Y flow component per unit area assigned to cell
F_{Y1} = flow component out of cell (at front face) in Y-direction
A_Y = area of cell (at front face) in Y-direction.

In the Z-direction (along layers):

$$F_Z = \frac{F_{Z1}}{A_Z} \tag{32}$$

where

F_Z = Z flow component per unit area assigned to cell
F_{Z1} = flow component out of cell (at lower face) in Z-direction
A_Z = area of cell (at lower face) in Z-direction.

Resultant three-dimensional flows per unit area ($F_{X\text{-}Y\text{-}Z}$) at model cells:

$$F_{X\text{-}Y\text{-}Z} = [(F_X)^2 + (F_Y)^2 + (F_Z)^2]^{1/2} \qquad (33)$$

Note that, flow direction for three-dimensional flows per unit area is not calculated in this version of POSTAIR. Also note that because flow values at the cell faces are used in the calculation of $F_{X\text{-}Y\text{-}Z}$, spatial coordinates reported in the output file represent values of cell centers. Output of $F_{X\text{-}Y\text{-}Z}$ is for all cells in the model domain and is oriented by layers. No option currently exists for specifying single layers nor for orienting output by row or column.

Resultant three-dimensional flows calculated for each cell in the model domain provide a useful means of predicting zones of influence of well or trench systems and their corresponding applied stresses. Output can be incorporated in three-dimensional graphical packages for visual presentation of flow magnitudes.

4.4 POSTAIR Convention for Naming Output Files

4.4.1 Output File Names for Single Parameters in Two-Dimensional Slices

As discussed in Section 4.3, the potential exists for a large number of output files to be generated by the postprocessor. To minimize the user input to the postprocessor, POSTAIR generates, within the program, file names for the output data. The output-file names are made up of combinations of letters and numbers that identify a feature of the output data. The convention used for generating file names is summarized below:

Output file name: abcdefgh.ijk

where

a = A for air-flow simulation, or
G for ground-water-flow simulation.

b = P for pressure output, or
H for head output, or
M for mass flow-rate output, or
V for volumetric flow-rate output.

c = C for center of cell, or
R for right face of cell, or
F for front face of cell, or
L for lower face of cell, or

c = I for resultant flow components in rows, or
J for resultant flow components in columns, or
K for resultant flow components in layers, or
U for resultant flow components per unit area in rows, or
V for resultant flow components per unit area in columns, or
W for resultant flow components per unit area in layers.

de = two-digit simulation identification number (specified by user).

f = X for row number, or
Y for column number, or
Z for layer number.

gh = two-digit row, column, or layer identification number (generated by program).

i = T for time step.

jk = two-digit time step identification number (generated by program).

To illustrate the output file names, consider the following examples:

- APC03X07.T01: is generated for output from an air-flow simulation (A), and quantifies pressure (P) at the center of the cell (C) of input data set (03), in model row (X) number (07), at time step (T) number (01).

- AMR01Z03.T02: is generated for output from an air-flow simulation (A), and quantifies mass flow rates (M) through the right-hand cell faces (R) of input data set (01), in model layer (Z) number (03), at time step (T) number (02).

- AVK04I05.T01: is generated for output from an air-flow simulation (A), and quantifies volumetric flow rates (V) for the two-dimensional resultant vectors (K) of input data set (04), in model row (I) number (05), at time step (T) number (01).

The above nomenclature generally is associated with multiple file output, with each file representing a single two-dimensional slice through the model domain. Because separate files also are generated for each of the nine possible output items, the maximum number of files that can be generated is nine times the number of layers, rows, or columns. Options to reduce the number of output files are discussed in Section 4.3.6.
Typical file contents for any slice will include:

- two spatial coordinates, one in each principal direction in the slice
- output item
- two nodal coordinates, one in each principal direction in the slice.

4.4.2 Output File Names for Combined Parameters in Two-Dimensional Slices

Files containing combined data at single, or at multiple, two-dimensional slices in the model domain are named within POSTAIR according to the following convention:

- PRESxx.Tyy — contains a listing of pressure-output data for cells in one or every two-dimensional slice in the model domain. Data are organized by layer only. Output is written in a text (ASCII) format. (PRESxx.Tyy applies to air-flow simulations only.)
- PRESxx.Byy — contains the same output as PRESxx.Tyy but data are written in a binary format. Data are organized by layer only. This option minimizes disk storage space but requires unformatted input to subsequent programs.
- HEADxx.Tyy — contains a listing of head-output data for cells in one or every two-dimensional slice in the model domain. Data are organized by layer only. Output is written in a text (ASCII) format. (HEADxx.Tyy applies to ground-water simulations only.)
- HEADxx.Byy — contains the same output as HEADxx.Tyy but data are written in a binary format organized by layer only. This option minimizes disk storage space but requires unformatted input to subsequent programs.
- FLOWVxx.Tyy — contains a listing of volumetric-flow-component output data for cells in one or every slice in the model domain. Data are organized by layer only. The file consists of four data subsets, namely net volumetric flows at constant-head cells (1); and volumetric flow components at active-cell right (2), front (3), and lower (4) faces. Output is written in a text (ASCII) format. (FLOWVxx.Tyy applies to air-flow and ground-water simulations.)
- FLOWVxx.Byy — contains the same output as FLOWVxx.Tyy but data are written in a binary format organized by layer only. This option minimizes disk storage space but requires unformatted input to subsequent programs.
- FLOWMxx.OUT — contains a listing of mass-flow-component output data for cells in single or multiple two-dimensional slices in the model domain. Data are organized by layer only. The file again consists of four data subsets, namely net mass flows at constant-head cells (1); and mass flow components at active-cell right (2), front (3), and lower (4) faces. Output is written in a text (ASCII) format. (FLOWVxx.Tyy applies to air-flow simulations only.)
- FLOWMxx.Byy — contains the same output as FLOWMxx.Tyy but data are written in a binary format organized by layer only. This option minimizes disk storage space but requires unformatted input to subsequent programs.

The xx in the file names represents the identification number specified by the user for the particular data set being analyzed. The yy in the file names represents the time step. Typical contents for the above files include:

- three spatial coordinates, one in each principal direction in the domain
- output item
- three nodal coordinates, one in each principal direction in the domain.

Disk storage requirements for output at every node location can be substantial. The binary output option can be used to minimize storage space.

4.4.3 Output File Names for Three-Dimensional Flow Resultants

Files containing resultant three-dimensional volumetric and mass flows per unit area at each cell in the model domain are named within POSTAIR according to the following convention:

- 3DQRVxx.Tyy — contains a listing of resultant three-dimensional volumetric flows per unit area at each cell in the model domain. Data are organized by layer only. Output is written in a text (ASCII) format.
- 3DQRMxx.Tyy — contains a listing of resultant three-dimensional mass flows per unit area at each cell in the model domain. Data are organized by layer only. Output is written in a text (ASCII) format.

The xx and yy in the file names have the same designation as that defined in the previous section. In addition, the contents for the above files are similar to those defined in the previous section.

4.4.4 Output File Names for Mass-Balance and Well Data

Files containing mass-balance, well, and unit data are named within POSTAIR according to the following convention:

MASSxx.Tyy contains mass-balance and well flows and pressure output calculated at the end of each time step. The unit system used in the air-flow simulation also is summarized in the MASSxx.Tyy file.

The xx in MASSxx represents the identification number specified by the user for the particular data set being analyzed. The yy in Tyy represents the simulation time step corresponding to the data output. Multiple files are generated during simulation with one file being written for each time step. Typical contents of the above file at the end of each time step include:

- mass flow through the atmospheric layer
- mass flow through the left, back, right, and front faces in the model domain

- total mass flow across model boundaries
- total mass flow through all wells and trenches in the model domain
- mass balance (mass in - mass out)
- percentage of air recharge from the atmosphere
- percentage of air recharge from lateral boundaries
- normalized mass balance (mass in - mass out)/total mass
- mass flow through individual wells and trenches
- volumetric flow through individual wells and trenches
- pressure in individual wells and trenches
- summary of the unit system used in the simulation.

4.5 POSTAIR Input and Output Files

4.5.1 POSTAIR Input Files

The files needed to implement the postprocessor, POSTAIR, for both air- and ground-water-flow simulations are summarized below. More detailed discussions of file formats and contents are presented in the sections referenced.

User-defined files:

- INFILEx.POS — used to specify the following--pneumatic or hydraulic simulation; coordinate system; spatial coordinate locations; head and (or) flow analysis; output by layer, row, or column; simulation identification number; single, multiple, and (or) resultant output files; complete or partial output; generation of mass balance output; two-dimensional slice; names of input files used by the postprocessor. INFILEx.POS is required to run POSTAIR in the direct-entry mode but can be neglected for interactive applications (Section 4.5.3).

MODFLOW input-data files:

- BASAIRx.PRN — MODFLOW Basic input file used to perform the simulation (Section 4.5.4).

- OCAIRx.PRN — MODFLOW Output-Control input file used to perform the simulation (Section 4.5.5).

- BCFAIRx.PRN — MODFLOW Block-Centered-Flow input file used to perform the simulation (Section 4.5.6).

MODFLOW output-data files:

- HEADx.BIN — MODFLOW binary output file storing head output from the simulation (Section 4.5.7).

- FLOWx.BIN — MODFLOW binary output file storing flow output from the simulation (Section 4.5.8).

Preprocessor/user-defined files:

- MODELx.DAT — a file storing unit selections, numbers of wells and trenches, certain physical data, depths of consecutive layer bottoms from a datum (or specified surface elevation), well/trench configurations, and well/trench pressures. This file is created by the air-flow preprocessor, PREAIR (Section 4.5.9).

INFILEx.POS is specified interactively by the user after invoking POSTAIR. The remaining files are read directly by POSTAIR. The available unit systems for air-flow simulations are discussed in Section 4.1.6. Selections of length, volume, time, pressure, temperature, mass, and permeability units should be consistent throughout the data entry. Data-output units will reflect those selected in the preprocessing stages.

4.5.2 POSTAIR Output Files

MODFLOW output files are modified by the postprocessor to obtain pressure, volumetric flow rates, and mass flow rates at selected cells in the model domain. A secondary function of POSTAIR is to organize output from air-flow simulations, according to user specifications. Five types of output can be produced by POSTAIR, as follows:

(1) output for pressure and (or) flow at single or multiple two-dimensional slices in the model domain (written to separate files in a text format; see Section 4.5.10);

(2) output for pressure and (or) flow at single or multiple two-dimensional slices in the model domain (written to single files in a text or binary format; see Section 4.5.11);

(3) output for one- and two-dimensional flow-rate resultants at single or multiple two-dimensional slices in the model domain (written to separate files in a text format; see Section 4.5.12);

(4) output for resultant three-dimensional flow-rates per unit area at each cell in the model domain (written to single files in a text format; see Section 4.5.13); and

(5) output for mass-balance and well-flow computations at the end of each time step (written to a single file in a text format; see Section 4.5.14).

4.5.3 POSTAIR Input File INFILEx.POS

File specification

Name of file:	Specified by the user after invoking the postprocessor (for example, INFILEx.POS). Note that POSTAIR also can be used interactively to setup or modify INFILEx.POS.
File contents:	Selections for the following: hydraulic or pneumatic analysis; coordinate system; spatial coordinate locations; pressure and (or) flow analysis, output by layer, row, or column; simulation identification numbers; single, multiple, and (or) resultant output; complete or partial output; two-dimensional slice; inclusion or omission of mass balance and well output; names of MODFLOW Basic, Output-Control, and Block-Centered-Flow input files; MODFLOW binary files with head- and flow-output data; and MODEL.DAT data transfer file.
File application:	This file is used to specify the type of analysis being performed and the names of input files associated with the postprocessor application.
Fortran unit number:	The program defines the INFILEx.POS input file a UNIT = 21.
Program input:	Input from INFILEx.POS is accomplished in the subroutine SETUP.

File structure

The structure of INFILEx.POS is as follows:

1. Data: IV(35),IV(36),IV(37),IV(38),IV(39),IV(40),IV(41),IV(42),IV(43)
   Format: 8I2,I4

2. Data: FNAME(3)
   Format: A12

3. Data: FNAME(4)
   Format: A12

4. Data: FNAME(5)
   Format: A12

5. Data: FNAME(7)
   Format: A12

6. Data: FNAME(8)
   Format: A12

7. Data: FNAME(9)
   Format: A12

Example input file--INFILE4.POS

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

1.    IV(35),IV(36),......,IV(42),IV(43)----- 2 1 1 2 2 4 3 1   3
2.    FNAME(3)--------------------------------BASAIR4.PRN
3.    FNAME(4)--------------------------------OCAIR4.PRN
4.    FNAME(5)--------------------------------BCFAIR4.PRN
5.    FNAME(7)--------------------------------HEAD4.BIN
6.    FNAME(8)--------------------------------FLOW4.BIN
7.    FNAME(9)--------------------------------MODEL4.DAT
```

Definition of INFILEx.POS variables

The definitions of input variables for the INFILEx.POS file are presented below. Variables are presented in the order in which they appear in the data file. Because information in the file consists of program-option settings and names of input and output files, no units are involved.

IV(35)

- IV(35) is the flag specifying whether simulation is hydraulic (IV(35)=1) or pneumatic (IV(35)=2). The definition of IV(35) does not appear in the MODFLOW documentation.
- IV(35) must be specified in order to implement POSTAIR.

IV(36)

- IV(36) is the flag specifying where the origins for the spatial and nodal coordinate systems are to be located (see Section 4.3.1). If IV(36)=1, then the origins of the spatial and nodal coordinate systems will coincide with the MODFLOW convention (upper-left-hand corner). If IV(36)=2, then the origin of the nodal coordinate system will coincide with the MODFLOW convention but the origin of the spatial coordinate system will be relocated to the lower-left-hand corner. If IV(36)=3, then the origins of both the nodal and spatial coordinate systems will be relocated to the lower-left-hand corner of the model domain.

Note that the application of IV(36) depends on the orientation of the output (controlled by IV(39)) specified by the user. Options IV(36)=1, IV(36)=2, and IV(36)=3 are all valid selections for output oriented by layers (IV(39)=1); however, only IV(36)=1 is allowed for output oriented by rows (IV(39)=2) and columns (IV(39)=3).

- IV(36) defaults to a value of 1 (retain the MODFLOW convention) when no value is specified by the user.

IV(37)

- IV(37) is the flag specifying the location of the spatial coordinates for flow rates at cell faces (see Section 4.3.2). MODFLOW calculates flow rates at the cell faces in the X-, Y- and Z-directions. For IV(37)=1, spatial coordinates at the cell faces will be generated for the flow rates. For IV(37)=2, spatial coordinates at the cell centers will be generated for the flow rates. IV(37)=1 gives an exact spatial output for the point of application, whereas IV(37)=2 gives an approximate spatial output for the point of application of the flow components. The approximate values can be useful in certain graphical packages. Note, however, that the selection of IV(37) does not change the computed value of the flow components. Note also that this option does not apply to head or pressure output, because these values always correspond to the cell-center coordinates.
- IV(37) defaults to a value of 1 (output spatial coordinates for flow rates at the cell faces) when no value is specified by the user.

IV(38)

- IV(38) is the flag specifying whether an analysis of pressure only (IV(38)=1), or pressure and flow (IV(38)=2), is to be performed (see Section 4.3.3). The selection of IV(38) affects all subsequent flow specifications. For example, a mass-balance and well-flow summary (specified by IV(42)=1) can be performed only if IV(38)=2. In air-flow simulations, when IV(38)=2, POSTAIR generates both mass and volumetric flow rates for selected slices.
- IV(38) defaults to a value of 2 (head/pressure simulation only) when no value is specified by the user.

IV(39)

- IV(39) is the flag specifying whether output from POSTAIR is oriented by layers (IV(39)=1), rows (IV(39)=2), or columns (IV(39)=3) (see Section 4.3.4). This option allows the user to organize output parameters by two-dimensional slices in plan or in section through the model domain.
- IV(39) defaults to a value of 1 (orient output by layers) when no value is specified by the user.

IV(40)

- IV(40) is a two-digit identification number assigned to the simulation by the user. The value of IV(40) appears in all the output file names and provides a method of cross-referencing output files with original data sets (see Section 4.4.1).
- IV(40) defaults to a value of 01 (ID # = 1 for simulation) when no value is specified by the user.

IV(41)

- IV(41) defines the format of the pressure and flow output (Section 4.3.5). For IV(41)=1, three TEXT files are generated--namely a pressure file, a volumetric flow file, and a mass flow file. Parameter locations are defined in the files by three spatial and three nodal coordinates.
  For IV(41)=-1, three BINARY files are generated--again, one pressure file, one volumetric flow file, and one mass flow file. Only parameter values are recorded in the binary files (no coordinate values).
  For IV(41)=2, multiple TEXT files are generated, with one file per pressure or flow parameter, per two-dimensional slice. Parameter locations are defined by two spatial and two nodal coordinates.
  For IV(41)=3, the TEXT files for IV(41)=2, along with two-dimensional RESULTANT flow files (see Section 4.3.7) are generated.
  For IV(41)=4, the TEXT files for IV(41)=2, along with three-dimensional RESULTANT flow files (see Section 4.3.7) are generated.
  The type of output depends on IV(38), which specifies head only, or head and flow output. Further, the extent of data contained in the output files is determined by the value of IV(43).
- IV(41) defaults to a value of 1 (write text output and do not generate two-dimensional resultant flow rates) when no value is specified by the user.

IV(42)

- IV(42) is the flag specifying whether a mass balance should be performed (IV(42)=1) or skipped (IV(42)=2) by POSTAIR. When specified, the mass balance is performed by using mass flow rates through constant-head cells. In air-flow simulations, all boundary cells are either constant-head cells or no-flow cells. Hence, flow rates at the lateral and atmospheric boundaries can be determined. No flow takes place through the lower (water-table) boundary. The postprocessor computes flow rates at the top (atmosphere) face, left face, back face, right face, front face, and wells and trenches. The flow rates are used to perform a mass balance.
- The percentage of air recharge from the atmosphere and the percentage of air recharge from the lateral domain also are calculated. All mass- balance data are written to a file MASSxx.Tyy, where xx represents the user-specified identification number for the simulation (IV(40)) and yy represents the time step. The mass-balance option is available only if the pressure and flow option (IV(38)=2) was specified by the user.
- IV(42) defaults to a value of 1 (perform mass balance) when no input value is specified by the user.

IV(43)

- IV(43) is the flag specifying whether to generate output at every (IV(43)=0) two-dimensional slice in the model domain or at a single layer (IV(43)=layer number), row (IV(43)=row number), or column (IV(43)=column number). IV(43) controls the data output to (1) single pressure and flow TEXT files (IV(41)=1), (2) single pressure and flow BINARY files (IV(41)=-1), (3) separate pressure and flow TEXT files (IV(41)=2), (4) separate pressure, flow, and two-dimensional resultant TEXT files (IV(41)=3), and (5) separate pressure, flow, and three-dimensional resultant TEXT files (IV(41)=4). For cases (1) and (2), three output file are generated. (Note that these files can only be oriented by layers (IV(39)=1). For cases (3) and (4), the number of output files depends on the value of IV(43). For IV(43)=0, the number of output files generated is nine times the number of layers, rows, or columns. For IV(43)>0, the number of output files generated is, at most, nine. (Note that these files can be oriented by layers IV(39)=1, rows IV(39)=2, or columns IV(39)=3). For case (3), two additional files per layer record two-dimensional flow resultants. For case (4), four additional files record three-dimensional flow resultants.

- IV(43) defaults to a value of 0 (output files are generated for every two-dimensional slice in the model domain oriented according to IV(39)) when no value is specified by the user.

FNAME(3)

- FNAME(3) is the name of the MODFLOW Basic (BAS) input file that contains air-flow data used to perform the simulation.
- FNAME(3) must be specified in order to implement POSTAIR.

FNAME(4)

- FNAME(4) is the name of the MODFLOW Output-Control (OC) input file that contains air-flow data used to perform the simulation.
- FNAME(4) must be specified in order to implement POSTAIR.

FNAME(5)

- FNAME(5) is the name of the MODFLOW Block-Centered-Flow (BCF) input file that contains air-flow data used to perform the simulation.
- FNAME(5) must be specified in order to implement POSTAIR.

FNAME(7)

- FNAME(7) is the name of the MODFLOW binary output file that contains head or pressure data generated during the simulation.
- FNAME(7) must be specified in order to implement POSTAIR.

FNAME(8)

- FNAME(8) is the name of the MODFLOW binary output file that contains flow data generated during the simulation.
- FNAME(8) must be specified only if flow analysis is being performed (IV(38)=2); otherwise, leave a blank line.

FNAME(9)

- FNAME(9) is the name of the file used to transfer selected model information between the pre- and postprocessors. The file name FNAME(9) is entered interactively into the postprocessor by the user.
- FNAME(9) defaults to the setting MODEL.DAT if no name is specified by the user. Note that a blank line must be left in the data file when no assignment is being made.

4.5.4 <u>POSTAIR Basic Input File BASAIRx.PRN</u>

The postprocessor extracts information from the MODFLOW Basic file (BASAIRx.PRN) and uses it to interpret the head and flow output. The name of the Basic data file is specified in the file INFILEx.POS and should be identical to that used to perform the MODFLOW simulation. BASAIRx.PRN is generated directly by the preprocessor PREAIR (Section 3.3.5) in air-flow simulations.

4.5.5 <u>POSTAIR Output-Control input file OCAIRx.PRN</u>

The postprocessor extracts information from the MODFLOW Output-Control file (OCAIRx.PRN) and determines the nature of the information written to the binary files. On the basis of the Output-Control data file, the postprocessor can evaluate the user requests for head and flow output against values generated during the MODFLOW simulation. If settings in the Output-Control file indicate that corresponding options selected by the user were not generated in the MODFLOW simulation, a warning to this effect is displayed on the screen. If the requested options conform to the Output-Control-file settings, the postprocessor proceeds with the run without interruption. The name of the Output-Control data file is specified in the file INFILEx.POS and should be identical to that used to perform the MODFLOW simulation. The contents and format of the file should match those in the original specifications used for the MODFLOW simulation. OCAIRx.PRN is generated directly by the preprocessor PREAIR (Section 3.3.6) in air-flow simulations.

4.5.6 <u>POSTAIR Block-Centered-Flow input file BCFAIRx.PRN</u>

The postprocessor extracts information from the Block-Centered-Flow file (BCFAIRx.PRN) and uses it to interpret the head and flow output. The name of the Block-Centered-Flow data file is specified in the file INFILEx.POS and should be identical to that used to perform the MODFLOW simulation. BCFAIRx.PRN is generated directly by the preprocessor PREAIR (Section 3.3.7) in air-flow simulations.

4.5.7 <u>POSTAIR Binary Head Output File HEADx.BIN</u>

File specifications

Name of file:	Specified by the user either directly by using INFILEx.POS or interactively. The file name must match the output-file name specified in the MODFLOW simulation.
File contents:	MODFLOW binary output containing head values (hydraulic simulations) or uncorrected pressure values (pneumatic simulations).
File application:	This file stores head or pressure data generated during applications of MODFLOW to ground-water or air-flow studies. To conserve space, MODFLOW writes out information in a binary format,

which must be converted back to a text format before being used to analyze a particular system.

Fortran unit number: The program defines the HEADx.BIN input file as UNIT = 17.

Parameter units: The unit system in the file corresponds to the selection made in defining the problem (see Basic and Block-Centered-Flow input data).

File structure

The structure of the binary head file output by MODFLOW and used as input for POSTAIR is as follows:

Input items 1 and 2 (head terms) for each time step and for each layer.

1. Data: KSTPH,KPERH,PERTIMH,TOTIMH,TEXTH,NHCOL,NHROW,NHLAY
   Format: Unformatted (Binary)

Input item 2 (head terms) for each row and column.

2. Data: BUFH(NHCOL,NHROW)
   Format: Unformatted (Binary)

Example Input File--HEADx.BIN

The format and contents of the output in the binary files are determined by the MODFLOW subroutine used to write the data set. All information contained in the binary file is generated by MODFLOW. The user must simply ensure that the necessary settings in the Output-Control file and Block-Centered-Flow files have been specified to generate the binary files. Consult MODFLOW documentation for additional details on binary output files.

Definition of Input Variables

The definitions of the input variables included in the HEADx.BIN file are presented below. Variables are presented in the order in which they appear in the data file. Where applicable, the unit system used in the binary file follows that used in the MODFLOW input file, such as the Basic and Block-Centered-flow files.

KSTPH

- KSTPH is the flag representing the time step corresponding to the head- output data set. The definition of KSTPH is the same as that of KSTP in the MODFLOW documentation.
- KSTPH is generated by MODFLOW if the Output-Control file is active (unit number assigned to Output-Control file in the Basic file) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

KPERH

- KPERH is the flag representing the stress period corresponding to the head-output data set. The definition of KPERH is the same as that of KPER in the MODFLOW documentation.
- KPERH is generated by MODFLOW if the Output-Control file is active (unit number assigned to the Output-Control file in the Basic file) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

PERTIMH

- PERTIMH records elapsed time in the stress period corresponding to the head-output data set.
- PERTIMH is generated by MODFLOW if the Output-Control file is active (unit number assigned to the Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

TOTIMH

- TOTIMH records elapsed time in the simulation up to the current head- output data set.
- TOTIMH is generated by MODFLOW if the Output-Control file is active (unit number assigned to the Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

TEXTH

- TEXTH is a label specified by MODFLOW corresponding to the head-output data set.
- TEXTH is generated by MODFLOW if the Output-Control file is active (unit number assigned to the Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

NHCOL

- NHCOL records the number of columns in the model domain.
- NHCOL is generated by MODFLOW if the Output-Control File is active (unit number assigned to the Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

NHROW

- NHROW records the number of rows in the model domain.
- NHROW is generated by MODFLOW if the Output-Control file is active (unit number assigned to Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

NHLAY

- NHLAY records the row layer number corresponding to the head-output data.
- NHLAY is generated by MODFLOW if the Output-Control file is active (unit number assigned to Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

BUFH(NHCOL,NHROW)

- BUFH is a two-dimensional array that contains head or pressure output from a MODFLOW simulation at each cell in the model domain.
- BUFH is generated by MODFLOW if the Output-Control file is active (unit number assigned to the Output-Control file in the Basic File) and IHEDUN>0, INCODE=0, IHDDFL>0, and Hdsv>0 have been specified.

4.5.8 POSTAIR Binary Flow Output File FLOWx.BIN

File specifications

Name of file:	Specified by user either directly by using INFILEx.POS or interactively. File name must match output-file name specified in the MODFLOW simulation.
File contents:	MODFLOW binary output containing flow values (hydraulic simulations) or uncorrected values used to compute volumetric and mass flow values (pneumatic simulations) at cell centers, right faces, front faces, and lower faces.
File application:	This file stores flow data generated during applications of MODFLOW to ground-water or air-flow studies. To conserve space, MODFLOW writes information to the file in a binary format, which must be converted back to a text format before being used to analyze a particular system.
Fortran unit number:	The program defines the FLOWx.BIN input file as UNIT = 18.
Program input:	Input from FLOWx.BIN is accomplished in the subroutine AFLOW.
Parameter units:	The unit system in the file corresponds to the selection made in defining the problem (see Basic and Block-Centered-Flow input data).

File Structure

The structure of the binary flow file output by MODFLOW and used as input for POSTAIR is as follows:

Input items 1 and 2 (flow terms) for each time step.
Input items 1 and 2 for each flow set (center, right, front, lower).

1. Data: KSTPF,KPERF,TEXTF,NFCOL,NFROW,NFLAY
   Format: Unformatted (Binary)

Input item 2 (head terms) for each layer, row, and column.

2. Data: BUFF(NFCOL,NFROW,NFLAY)
   Format: Unformatted (Binary)

Example Input File--FLOWx.BIN

The format and contents of the output in the binary files are determined by the MODFLOW subroutine used to write the data set. All information contained in the binary file is generated by MODFLOW. The user must simply ensure that the necessary settings in the Output-Control file and Block-Centered-Flow file have been specified to generate the binary files. Consult MODFLOW documentation for additional details on binary output files.

Definition of Input Variables

The definitions of the input variables included in the FLOWx.BIN file are presented below. Variables are presented in the order in which they appear in the data file. Where applicable, the unit system used in the binary file is the same as that used in the MODFLOW input file, such as the Basic and Block-Centered-flow files.

KSTPF

- KSTPF is the flag representing the time step corresponding to the flow- output data set.
- KSTPF is generated by MODFLOW, if the Output-Control and Block-Centered-Flow files are active (unit numbers assigned to these files in the Basic File) and INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

KPERF

- KPERF is the flag for the stress period.
- KPERF is generated by MODFLOW, if the Output-Control and Block-Centerd-Flow files are active (unit numbers assigned to Output-Control and Block-Centered-Flow files in the Basic File), INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

TEXTF

- TEXTF is a label specified by MODFLOW corresponding to the flow-output data set.
- TEXTF is generated by MODFLOW, if the Output-Control and Block-Centerd-Flow files are active (unit numbers assigned to Output-Control and Block-Centerd-Flow files in the Basic File), INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

NFCOL

- NFCOL records the number of columns in the model domain.
- NFCOL is always generated by MODFLOW, providing that the Output-Control and Block-Centerd-Flow files are active (unit numbers assigned to Output-Control and Block-Centerd-Flow files in the Basic file), INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

NFROW

- NFROW records the number of rows in the model domain.
- NFROW is always generated by MODFLOW, providing that the Output-Control and Block-Centered-Flow files are active (unit numbers assigned to Output-Control and Block-Centered-Flow files in the Basic file), and INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

NFLAY

- NFLAY records the layer number corresponding to the flow-output data set.
- NFLAY is generated by MODFLOW, if the Output-Control and Block-Centered-Flow files are active (unit numbers assigned to the Output-Control and Block-Centered-Flow files in the Basic file), INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

BUFF(NFCOL,NFROW,NFLAY)

- BUFF is a three-dimensional array containing flow output from a MODFLOW simulation at center, right, front, and lower faces of cells.
- BUFF is generated by MODFLOW if, the Output-Control and Block-Centered-Flow files are active (unit numbers assigned to Output-Control and Block-Centerd-Flow files in the Basic file), INCODE=0 and ICBCFL>0 have been specified in the Output-Control file, and IBCFCB>0 has been specified in the Block-Centered-Flow file.

4.5.9 <u>POSTAIR Model Data Output File MODEL.DAT</u>

The postprocessor uses data stored in the MODEL.DAT file to generate vertical spatial coordinates for output parameters. In addition, for air-flow simulations, physical constants such as the thickness of the superimposed atmospheric layer (in the Z-direction) and air temperature are retrieved from the MODEL.DAT file. Information on well and trench locations and pressures also are recorded in the MODEL.DAT file. The data requirements for the file do not appear in the MODFLOW Users' Manual. Details of the file format and contents are presented in Section 3.3.10.

The MODEL.DAT file must be present when POSTAIR is invoked. The file is generated automatically by the air-flow preprocessor PREAIR; however, when POSTAIR is used independently of PREAIR, the user must set up MODEL.DAT manually. The name of the MODEL.DAT file is specified within both the pre- and postprocessor input files. The file name should remain constant throughout the air-flow simulation.

4.5.10 POSTAIR Head and Flow Output Files for Two-Dimensional Slices

File specification

Name of files:	Multiple files (minimum of nine, maximum of nine times NLAY, or nine times NROW, or nine times NCOL) are generated and named by POSTAIR according to the convention described in Section 4.4.
File contents:	One file is generated per output item per two-dimensional slice, depending on the values for IV(38) and IV(43) (see Section 4.5.3). Output parameters for an air-flow simulation can include pressure at cell centers, volumetric flow rate at constant-head cells, volumetric flow rate through right face of cells, volumetric flow rate through front face of cells, volumetric flow rate through lower face of cells, mass flow rate at constant-head cells, mass flow rate through right face of cells, mass flow rate through front face of cells, and mass flow rate through lower face of cells. Output parameters for ground-water simulations are similar to those for air flow, except that pressure output is replaced with hydraulic head and there is no output for mass flow. Two-dimensional slices can be oriented by layer, row, or column, depending on the value of IV(39).
File application:	These files record the head and flow output in a two-dimensional slice in the model domain as well as spatial and nodal coordinates in the two principal directions.
Fortran unit number:	The program outputs pressure to files as UNIT=28, volumetric flow rates to files as UNIT=29, and mass flow rates to files as UNIT=30.
Program output:	Output to the pressure and flow files is accomplished in the subroutines PRES and AFLOW.
Physical units:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output are specified by the user when entering data into the preprocessor. Output units correspond to units used for input data. If no unit system was specified, output units conform to the default unit system.

File Structure

The structure of the head/pressure- and flow- output files for two -dimensional slices is as follows. Item 1 is output (NROW)(NCOL) times for sorts by layer, or (NLAY)(NCOL) times for sorts by row, or (NLAY)(NROW) times for sorts by column.

1. Data: CD1,CD2,COR,ND1,ND2
   Format: 2F15.5,E20.8,2I5

Note that, for pressure and flow output sorted by layer, a maximum of nine times (NLAY) files can be generated; for output sorted by row, nine times NROW files can be generated; and for output sorted by column, nine times NCOL files can be generated (one file per output item per two-dimensional slice). Alternatively, the user can specify that files for each parameter are generated for a single two-dimensional slice oriented by layer, row, or column. Output-file names are generated directly by POSTAIR according to the convention described in Section 4.4.

Example Output Files

Values specified in the POSTAIR input file INFILEx.POS control the nature and extent of the simulation output. For example, the values specified in the input file listed in Section 4.5.3 require that:

- pressure and flow output (IV(38)=2) be generated for the air-flow simulation (IV(35)=2)
- output be oriented by rows (IV(39)=2) and generated for a single two-dimensional slice (row 3, IV(43)=3)
- spatial and nodal coordinates conform with MODFLOW convention (IV(36)=1)
- spatial coordinates for flow rates are output at cell faces (IV(37)=1)
- the simulation identification number is 04 (IV(40)=04).

For the values listed in data item 1 for the example input file in Section 4.5.3, the following two-dimensional parameter output files are generated for time step 1 (T01) and simulation number 4 (04):

- APC04X03.T01 pressure output at cell centers in row 3
- AVC04X03.T01 volumetric flow rates at constant-head cells in row 3
- AVR04X03.T01 volumetric flow rates at right faces of cells in row 3
- AVF04X03.T01 volumetric flow rates at front faces of cells in row 3
- AVL04X03.T01 volumetric flow rates at lower faces of cells in row 3
- AMC04X03.T01 mass flow rates at constant head cells in row 3
- AMR04X03.T01 mass flow rates at right faces of cells in row 3
- AMF04X03.T01 mass flow rates at front faces of cells in row 3
- AML04X03.T01 mass flow rates at lower faces of cells in row 3.

Contents of three of the above files are presented below to illustrate output data. The files presented are APC04X03.T01 (pressure output), AVC04X03.T01 (volumetric-flow-rate output at constant-head cells), and AMR04X03.T01 (mass-flow-rate output through right faces of active cells).

Pressure output at cell centers in row 3, contained in the file APC04X03.T01, is presented below.

Output records

1 5 10 15 20 25 30 35 40 45 50 55 60

Data item	Explanation					
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	10.00000	.10000000E+01	1	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	10.00000	.10000000E+01	2	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	10.00000	.10000000E+01	3	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	10.00000	.10000000E+01	4	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	10.00000	.10000000E+01	5	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	10.00000	.10000000E+01	6	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	10.00000	.10000000E+01	7	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-50.00000	.10000000E+01	1	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-50.00000	.99996920E+00	2	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-50.00000	.99991230E+00	3	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-50.00000	.10002070E+04	4	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-50.00000	.99991230E+00	5	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-50.00000	.99996920E+00	6	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-50.00000	.10000000E+01	7	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-150.00000	.10000000E+01	1	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-150.00000	.98837140E+00	2	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-150.00000	.96537800E+00	3	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-150.00000	.90000000E+00	4	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-150.00000	.96537800E+00	5	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-150.00000	.98837140E+00	6	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-150.00000	.10000000E+01	7	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-250.00000	.10000000E+01	1	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-250.00000	.99814400E+00	2	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-250.00000	.99602710E+00	3	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-250.00000	.99405070E+00	4	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-250.00000	.99602710E+00	5	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-250.00000	.99814400E+00	6	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-250.00000	.10000000E+01	7	3

Volumetric-flow-rate output at constant-head cells in row 3, contained in the file AVC04X03.T01, is presented below.

Data item	Explanation	Output records (columns 1–60)				
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	10.00000	.00000000E+00	1	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	10.00000	.88606950E+01	2	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	10.00000	.25243290E+02	3	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	10.00000	.00000000E+00	4	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	10.00000	.25243290E+02	5	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	10.00000	.88606950E+01	6	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	10.00000	.00000000E+00	7	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-50.00000	.17721390E+00	1	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-50.00000	.00000000E+00	2	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-50.00000	.00000000E+00	3	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-50.00000	.00000000E+00	4	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-50.00000	.00000000E+00	5	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-50.00000	.00000000E+00	6	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-50.00000	.17721390E+00	7	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-150.00000	.13310940E+03	1	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-150.00000	.00000000E+00	2	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-150.00000	.00000000E+00	3	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-150.00000	-.33055740E+04	4	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-150.00000	.00000000E+00	5	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-150.00000	.00000000E+00	6	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-150.00000	.13310940E+03	7	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	50.00000	-250.00000	.21348810E+02	1	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	150.00000	-250.00000	.00000000E+00	2	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	250.00000	-250.00000	.00000000E+00	3	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	350.00000	-250.00000	.00000000E+00	4	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	450.00000	-250.00000	.00000000E+00	5	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	550.00000	-250.00000	.00000000E+00	6	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	650.00000	-250.00000	.21348810E+02	7	3

Mass-flow-rate output at right faces of cells in row 3, contained in the file AMR04X03.T01, is presented below. Note that spatial coordinates reflect the locations of the right faces of cells because IV(37)=1.

Data item	Explanation	Output records				
		1 5 10 15 20 25 30 35 40 45 50 55 60				
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	100.00000	10.00000	.00000000E+00	1	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	200.00000	10.00000	.00000000E+00	2	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	300.00000	10.00000	.00000000E+00	3	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	400.00000	10.00000	.00000000E+00	4	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	500.00000	10.00000	.00000000E+00	5	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	600.00000	10.00000	.00000000E+00	6	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	700.00000	10.00000	.00000000E+00	7	0
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	100.00000	-50.00000	.21966400E-03	1	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	200.00000	-50.00000	.40613830E-03	2	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	300.00000	-50.00000	.00000000E+00	3	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	400.00000	-50.00000	.00000000E+00	4	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	500.00000	-50.00000	-.40613830E-03	5	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	600.00000	-50.00000	-.21966400E-03	6	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	700.00000	-50.00000	.00000000E+00	7	1
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	100.00000	-150.00000	.16499470E+00	1	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	200.00000	-150.00000	.32056350E+00	2	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	300.00000	-150.00000	.87024620E+00	3	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	400.00000	-150.00000	-.87024620E+00	4	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	500.00000	-150.00000	-.32056350E+00	5	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	600.00000	-150.00000	-.16499470E+00	6	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	700.00000	-150.00000	.00000000E+00	7	2
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	100.00000	-250.00000	.26462740E-01	1	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	200.00000	-250.00000	.30124200E-01	2	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	300.00000	-250.00000	.28066500E-01	3	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	400.00000	-250.00000	-.28066500E-01	4	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	500.00000	-250.00000	-.30124200E-01	5	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	600.00000	-250.00000	-.26462740E-01	6	3
1.	CD1,CD2,COR,ND1,ND2————(row 3)——	700.00000	-250.00000	.00000000E+00	7	3

Definition of Variables

The definitions of variables output to the two-dimensional parameter files are presented below. Variables are presented in the order in which they appear in the data file. Units in the output file correspond to those in the original specifications.

CD1

- CD1 is the first of two spatial coordinates that define the application point of an output item in a two-dimensional slice. For head/pressure output and flow at constant-head cells, CD1 represents the distance from a specified origin to the center of the cell. For flow at cell faces, CD1 represents either the distance to the cell face or the distance to the cell center from a specified origin, depending on the value of IV(37) specified in the POSTAIR input file INFILEx.POS. The location of the spatial- and nodal-coordinate origins is controlled by the variable IV(36) in INFILEx.POS. If output is by layers or rows, CD1 will correspond to the distance along a row (in the X-direction). If output is by columns, CD1 will correspond to the distance along a column (in the Y-direction).
- CD1 is always present in the files that record parameter output for two-dimensional slices in the model.

CD2

- CD2 is the second of two spatial coordinates that define the point of application of an output item in a two-dimensional slice. For head/ pressure output and flow at constant-head cells, CD2 represents the distance from a specified origin to the center of the cell. For flow at cell faces, CD2 represents either the distance to the cell face or the distance to the cell center from a specified origin, depending on the value of IV(37) specified in the POSTAIR input file INFILEx.POS. The location of the spatial- and nodal-coordinate origins is controlled by the variable IV(36) in INFILEx.POS. If output is by layers, CD2 will correspond to the distance along a column (in the Y-direction). If output is by rows or columns, CD2 will correspond to the distance along a layer (in the Z-direction), generated from data contained in the MODEL.DAT file.
- CD2 is always present in the files that record parameter output for two-dimensional slices in the model.

COR

- COR is the output item at each cell location in a two-dimensional slice. One file with COR values is generated for each output item for each two-dimensional slice in the model, depending on values for IV(38) and IV(43) in the POSTAIR input file INFILEx.POS. Output items for an air-flow simulation can include pressure at cell centers, volumetric flow rate at constant-head cells, volumetric flow rate through right face of cells, volumetric flow rate through front face of cells, volumetric flow rate through lower face of cells, mass flow rate at constant-head cells, mass flow rate through right face of cells, mass flow rate through front face of cells, and mass flow rate through lower face of cells. Two-dimensional slices can be by layer, row, or column, depending on the value of IV(36) in INFILEx.POS.
- COR is always present in the files that record parameters output for two-dimensional slices in the model.

ND1

- ND1 is the first of two nodal coordinates that define the layer, row, or column number corresponding to the output parameter for a two-dimensional slice. The location of the spatial- and nodal-coordinate origins is controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. If output is by layers or rows, ND1 will correspond to the column number. If output is by columns, ND1 will correspond to the row number.
- ND1 is always present in the files that record parameter output for two-dimensional slices in the model.

ND2

- ND2 is the second of two nodal coordinates that define the layer, row, or column number corresponding to the output parameter for a two-dimensional slice. The location of the spatial- and nodal-coordinate origins is controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. If output is by layers, ND2 will correspond to the row numbers. If output is by rows or columns, ND2 will correspond to the layer number.
- ND2 is always present in the files that record parameter output for two-dimensional slices in the model.

4.5.11 POSTAIR Combined Head and Flow Output Files for Two-Dimensional Slices

File specification

Name of files:	A maximum of three files per time step can be generated. These files are named by POSTAIR according to the convention described in Section 4.4 (PRESxx.T01, FLOWVxx.T01, and FLOWMxx.T01 for text output, or PRESxx.B01, FLOWVxx.B01, and FLOWMxx.B01 for binary output).
File contents:	One file is generated for head/pressure output for single or multiple two-dimensional slices in the model domain. A second file is generated for volumetric flow rates at constant-head cells, and at right faces, front faces, and lower faces of active cells, in single or multiple two-dimensional slices in the model domain. A third file is generated for mass flow rates at constant-head cells, and at right faces, front faces, and lower faces of active cells, in single or multiple two-dimensional slices in the model domain. Single or multiple slices in the output files depend on the value of IV(43) in INFILEx.POS. Two-dimensional slices can be oriented by layer, row, or column depending on the value of IV(36) in INFILEx.POS.
File application:	These files record the head and flow output in two-dimensional slices in the model domain as well as spatial and nodal coordinates in the two principal directions.

Fortran unit:	The program outputs pressure to files as UNIT=25, volumetric flow rates to files as UNIT=26, and mass flow rates to files as UNIT=27.
Program output:	Output to the pressure and flow files is accomplished in the subroutines PRES AND AFLOW.
Physical units:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability are specified when the data are entered into the preprocessor. If no unit system was specified, output units conform to the default unit systems for each parameter.

File Structure

The structure of the head/pressure- and flow-output files for two-dimensional slices is as follows. Item 1 is output (I1)(I2)(NROW)(NCOL) times for sorts by layer, or (I1)(I2)(NLAY)(NCOL) times for sorts by row, or (I1)(I2)(NLAY)(NROW) times for sorts by column.

1. Data: CC1,CC2,CC3,COR,NC1,NC2,NC3
   Format: 3F15.5,E20.8,3I5

where I1=1 for head/pressure output and I1=4 for flow output. For IV(43)≠0 (a single two-dimensional slice is output), I2=1. For IV(43)=0 (every two-dimensional slice is output), I2=NLAY for output by layers, I2=NROW for output by rows, and I2=NCOL for output by columns. A maximum of three files per time step can be generated (one for head/pressure output, one for combined volumetric-flow-rate output, and one for combined mass-flow-rate output) depending on the value of IV(38). Output-file names are generated directly by POSTAIR according to the convention described in Section 4.4.

Example Output Files

Settings specified in the POSTAIR input file INFILEx.POS control the nature and extent of the simulation output. For example, the values specified in item 1 of the example input file listed in Section 4.5.3 require that:

- pressure and flow output (IV(38)=2) be generated for the air-flow simulation (IV(35)=2)
- multiple output files for pressure and flow output (IV(41)=3) are created
- output is oriented by rows (IV(39)=2) and generated for a single two-dimensional slice (row 3, IV(43)=3)
- spatial and nodal coordinates conform with MODFLOW convention (IV(36)=1)
- spatial coordinates for flow rates are at cell faces (IV(37)=1)
- the simulation identification number is 04 (IV(40)=04).

By specifying the value IV(41)=1 in the input file listed in Section 4.5.3, the following two-dimensional combined parameter output files are generated for time step 1 (T01) and simulation number 4 (04):

- PRES04.T01 — pressure output in row 3, at cell centers, with three-dimensional spatial and nodal coordinates;
- FLOWV04.T01 — volumetric-flow-rate output in row 3, at the centers of constant-head cells, right faces of active cells, front faces of active cells, and lower faces of active cells, along with three-dimensional spatial and nodal coordinates;
- FLOWM04.T01 — mass-flow-rate output in row 3, at the centers of constant-head cells, right faces of active cells, front faces of active cells, and lower faces of active cells, along with three-dimensional spatial and nodal coordinates.

Contents of two of the above files are presented below to illustrate output data. The files presented are PRES04.T01 (pressure output) and FLOWM04.T01 (combined mass-flow-rate output). Note that the above output also can be written in a binary format by specifying IV(41) = -1 in INFILEx.POS.

Combined pressure output at cell centers, in row 3, is contained in the file PRES04.T01, and an example is presented below.

```
                                              Output records
Data        Explanation     |---+----+----+----+----+----+----+----+----+----+----+----+----+----+----+----+
item                        1   5   10   15   20   25   30   35   40   45   50   55   60   65   70   75   80

 1.  CC1,...,NC3---(row 3)-      50.00000     250.00000      10.00000      .10000000E+01   1    3    0
 1.  CC1,...,NC3---(row 3)-     150.00000     250.00000      10.00000      .10000000E+01   2    3    0
 1.  CC1,...,NC3---(row 3)-     250.00000     250.00000      10.00000      .10000000E+01   3    3    0
 1.  CC1,...,NC3---(row 3)-     350.00000     250.00000      10.00000      .10000000E+01   4    3    0
 1.  CC1,...,NC3---(row 3)-     450.00000     250.00000      10.00000      .10000000E+01   5    3    0
 1.  CC1,...,NC3---(row 3)-     550.00000     250.00000      10.00000      .10000000E+01   6    3    0
 1.  CC1,...,NC3---(row 3)-     650.00000     250.00000      10.00000      .10000000E+01   7    3    0
 1.  CC1,...,NC3---(row 3)-      50.00000     250.00000     -50.00000      .10000000E+01   1    3    1
 1.  CC1,...,NC3---(row 3)-     150.00000     250.00000     -50.00000      .99996920E+00   2    3    1
 1.  CC1,...,NC3---(row 3)-     250.00000     250.00000     -50.00000      .99991230E+00   3    3    1
 1.  CC1,...,NC3---(row 3)-     350.00000     250.00000     -50.00000      .10002070E+04   4    3    1
 1.  CC1,...,NC3---(row 3)-     450.00000     250.00000     -50.00000      .99991230E+00   5    3    1
 1.  CC1,...,NC3---(row 3)-     550.00000     250.00000     -50.00000      .99996920E+00   6    3    1
 1.  CC1,...,NC3---(row 3)-     650.00000     250.00000     -50.00000      .10000000E+01   7    3    1
```

Data item	Explanation	Output records						
1.	CC1,...,NC3—(row 3)–	50.00000	250.00000	-150.00000	.10000000E+01	1	3	2
1.	CC1,...,NC3—(row 3)–	150.00000	250.00000	-150.00000	.98837140E+00	2	3	2
1.	CC1,...,NC3—(row 3)–	250.00000	250.00000	-150.00000	.96537800E+00	3	3	2
1.	CC1,...,NC3—(row 3)–	350.00000	250.00000	-150.00000	.90000000E+00	4	3	2
1.	CC1,...,NC3—(row 3)–	450.00000	250.00000	-150.00000	.96537800E+00	5	3	2
1.	CC1,...,NC3—(row 3)–	550.00000	250.00000	-150.00000	.98837140E+00	6	3	2
1.	CC1,...,NC3—(row 3)–	650.00000	250.00000	-150.00000	.10000000E+01	7	3	2
1.	CC1,...,NC3—(row 3)–	50.00000	250.00000	-250.00000	.10000000E+01	1	3	3
1.	CC1,...,NC3—(row 3)–	150.00000	250.00000	-250.00000	.99814400E+00	2	3	3
1.	CC1,...,NC3—(row 3)–	250.00000	250.00000	-250.00000	.99602710E+00	3	3	3
1.	CC1,...,NC3—(row 3)–	350.00000	250.00000	-250.00000	.99405070E+00	4	3	3
1.	CC1,...,NC3—(row 3)–	450.00000	250.00000	-250.00000	.99602710E+00	5	3	3
1.	CC1,...,NC3—(row 3)–	550.00000	250.00000	-250.00000	.99814400E+00	6	3	3
1.	CC1,...,NC3—(row 3)–	650.00000	250.00000	-250.00000	.10000000E+01	7	3	3

Combined mass-flow-rate output at cell centers in constant-head cells, at right faces of active cells, at front faces of active cells, and at lower faces of active cells in row 3, is contained in the file FLOWM04.T01. Part of a file is presented below.

Data item	Explanation	Output records (mass flow rate at constant head cells)						
1.	CC1,...,NC3—(row 3)–	50.00000	250.00000	10.00000	.00000000E+00	1	3	0
1.	CC1,...,NC3—(row 3)–	150.00000	250.00000	10.00000	.10983200E-01	2	3	0
1.	CC1,...,NC3—(row 3)–	250.00000	250.00000	10.00000	.31290110E-01	3	3	0
1.	CC1,...,NC3—(row 3)–	350.00000	250.00000	10.00000	.00000000E+00	4	3	0
1.	CC1,...,NC3—(row 3)–	450.00000	250.00000	10.00000	.31290110E-01	5	3	0
1.	CC1,...,NC3—(row 3)–	550.00000	250.00000	10.00000	.10983200E-01	6	3	0
1.	CC1,...,NC3—(row 3)–	650.00000	250.00000	10.00000	.00000000E+00	7	3	0
1.	CC1,...,NC3—(row 3)–	50.00000	250.00000	-50.00000	.21966400E-03	1	3	1
1.	CC1,...,NC3—(row 3)–	150.00000	250.00000	-50.00000	.00000000E+00	2	3	1

Output records (mass flow rate at constant head cells)

Data item	Explanation	1 — 15	20 — 30	35 — 45	50 — 65	70	75	80
1.	CC1,...,NC3—(row 3)-	250.00000	250.00000	-50.00000	.00000000E+00	3	3	1
1.	CC1,...,NC3—(row 3)-	350.00000	250.00000	-50.00000	.00000000E+00	4	3	1
1.	CC1,...,NC3—(row 3)-	450.00000	250.00000	-50.00000	.00000000E+00	5	3	1
1.	CC1,...,NC3—(row 3)-	550.00000	250.00000	-50.00000	.00000000E+00	6	3	1
1.	CC1,...,NC3—(row 3)-	650.00000	250.00000	-50.00000	.21966400E-03	7	3	1
1.	CC1,...,NC3—(row 3)-	50.00000	250.00000	-150.00000	.16499470E+00	1	3	2
1.	CC1,...,NC3—(row 3)-	150.00000	250.00000	-150.00000	.00000000E+00	2	3	2
1.	CC1,...,NC3—(row 3)-	250.00000	250.00000	-150.00000	.00000000E+00	3	3	2
1.	CC1,...,NC3—(row 3)-	350.00000	250.00000	-150.00000	-.36876570E+01	4	3	2
1.	CC1,...,NC3—(row 3)-	450.00000	250.00000	-150.00000	.00000000E+00	5	3	2
1.	CC1,...,NC3—(row 3)-	550.00000	250.00000	-150.00000	.00000000E+00	6	3	2
1.	CC1,...,NC3—(row 3)-	650.00000	250.00000	-150.00000	.16499470E+00	7	3	2
1.	CC1,...,NC3—(row 3)-	50.00000	250.00000	-250.00000	.26462740E-01	1	3	3
1.	CC1,...,NC3—(row 3)-	150.00000	250.00000	-250.00000	.00000000E+00	2	3	3
1.	CC1,...,NC3—(row 3)-	250.00000	250.00000	-250.00000	.00000000E+00	3	3	3
1.	CC1,...,NC3—(row 3)-	350.00000	250.00000	-250.00000	.00000000E+00	4	3	3

Definition of Output Variables

The definitions of variables output to the two-dimensional combined parameter files are presented below. Variables are presented in the order in which they appear in the data file. Units in the output file correspond to original specifications.

CC1

- CC1 is the first of three spatial coordinates that define the point of application of an output parameter in a two-dimensional slice. For head/ pressure output and flow at constant-head cells, CC1 represents the distance from a specified origin along a row (in the X-direction) to the center of the cell at which the parameters act. For flow at cell faces, CC1 represents either the distance along a row to the right cell face, or the distance along a row to the cell center from a specified origin, depending on the value of IV(37) set in the POSTAIR input file INFILEx.POS. The locations of the spatial- and nodal-coordinate origins are controlled by the variable IV(36) in INFILEx.POS. CC1 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).
- CC1 is always present in the files that record combined parameter output for two-dimensional slices in the model.

CC2

- CC2 is the second of three spatial coordinates that define the point of application of an output parameter in a two-dimensional slice. For head/ pressure output and flow at constant-head cells, CC2 represents the distance from a specified origin along a column (in the Y-direction) to the center of the cell at which the parameters act. For flow at cell faces, CC2 represents either the distance along a column to the front cell face, or the distance along a column to the cell center from a specified origin, depending on the value of IV(37) in the POSTAIR input file INFILEx.POS. The locations of the spatial and nodal coordinate origins are controlled by the variable IV(36) in INFILEx.POS. CC2 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).
- CC2 is always present in the files that record combined parameters output for two-dimensional slices in the model.

CC3

- CC3 is the third of three spatial coordinates that define the point of application of an output parameter in a two-dimensional slice. For head/ pressure output and flow at constant-head cells, CC3 represents an elevation (in the Z-direction relative to the ground-surface elevation specified in the MODEL.DAT file) of the center of the cell at which the parameters act. For flow at cell faces, CC3 represents either the elevation of the lower cell face, or the elevation of the cell center, depending on the value of IV(37) set in the POSTAIR input file INFILEx.POS. CC3 depends on the ground-surface elevation GELEV specified in the MODEL.DAT file. CC3 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).
- CC3 is always present in the files that record combined parameter output for two-dimensional slices in the model.

COR

- COR is the output parameter at each cell location in a two-dimensional slice. One file with COR values is generated for head/pressure output for single or multiple two-dimensional slices in the model, depending on values of IV(43) in the POSTAIR input file INFILEx.POS. A second file with COR values is generated for volumetric-flow-rate output at centers of constant-head cells, and at right, front, and lower cell faces of active cells, for single or multiple two-dimensional slices, depending on values of IV(38) and IV(43). For air-flow simulations, a third file with COR values is generated for mass-flow-rate output at centers of constant-head cells, and at right, front, and lower cell faces of active cells, for single or multiple two-dimensional slices, depending on values of IV(35), IV(38), and IV(43).
- COR is always present in the files that record combined parameter output for single or multiple two-dimensional slices in the model.

NC1

- NC1 is a nodal coordinate that defines the column number corresponding to the output parameter for a two-dimensional slice. The locations of the spatial and nodal coordinate origins are controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. NC1 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).

- NC1 is always present in the files that record combined parameter output for single or multiple two-dimensional slices in the model.

NC2

- NC2 is a nodal coordinate that defines the row number corresponding to the output parameter for a two-dimensional slice. The location of the spatial and nodal coordinate origins is controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. NC2 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).
- NC2 is always present in the files that record combined parameter output for single or multiple two-dimensional slices in the model.

NC3

- NC3 is a nodal coordinate that defines the layer number corresponding to the output parameter for a two-dimensional slice. The locations of the spatial and nodal coordinate origins are controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. NC3 does not depend on the selection made for orientation of the output (variable IV(39) in INFILEx.POS).
- NC3 is always present in the files that record combined parameter output for single or multiple, two-dimensional slices in the model.

4.5.12 POSTAIR Resultant Flow Output Files for Two-Dimensional Slices

File Specification

Name of files:	One file for two-dimensional resultant volumetric flow rates and one file for two-dimensional resultant mass flow rates are generated (depending on the value of IV(41)) for each two-dimensional slice in the domain specified by the user (depending on the value of IV(43)). A minimum of two, or a maximum of two times NLAY, or two times NROW, or two times NCOL files can be generated. Each file is named directly by POSTAIR according to the convention described in Section 4.4.
File contents:	The files contain the locations, directions, and magnitudes of resultant flow rates at each cell location in a selected two-dimensional slice through the model. For pneumatic simulations, flow rates for volumetric and mass flow are produced. For ground-water-flow simulations, only volumetric rates flow are produced.
File application:	These files record resultant volumetric- and mass-flow-rate output generated by POSTAIR from orthogonal components in a two-dimensional slice in the model.

Program output: Output to the head/pressure and flow files is accomplished in the subroutine R2FLOW.

Physical units: Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output are specified by the user when data are entered into the preprocessor. Output units correspond to initial settings. If no unit system was specified, output units conform to the default unit systems for each parameter.

File Structure

The structure of the head/pressure- and flow-output files for two-dimensional slices is as follows. Item 1 is output (NROW)(NCOL) times for sorts by layer, or (NLAY)(NCOL) times for sorts by row, or (NLAY)(NROW) times for sorts by column.

1. Data: CR1,CR2,FA1,FA2,FR1,FD1,NR1,NR2
   Format: 2F10.2,3E15.6,F10.2,2I5

Note that, for flow output sorted by layer, a maximum of two times NLAY files can be generated; for output sorted by row, two times NROW files can be generated; and for output sorted by column, two times NCOL files can be generated. Alternatively, the user can specify that files for each resultant flow rate be generated for a single two-dimensional slice oriented by layer, row, or column. Output-file names are generated directly by POSTAIR according to the convention described in Section 4.4.

Example Output File

Values specified in the POSTAIR input file INFILEx.POS control the nature and extent of the simulation output. For example, the values specified in the input file listed in Section 4.5.3 require that:

- pressure and flow output (IV(38)=2) be generated for the air-flow simulation (IV(35)=2)
- output is by rows (IV(39)=2) and generated for a single two-dimensional slice (row 3, IV(43)=3)
- spatial and nodal coordinates conform with MODFLOW convention (IV(36)=1)
- flow-rate resultants are generated (IV(41)=3) and spatial coordinates for flow rates at cell faces reflect cell faces (IV(37)=1)
- simulation identification number is 4 (IV(40)=04).

For the settings given in Section 4.5.3, the following two-dimensional output files are generated for time step 1 (T01) and simulation number 4 (04):

- AVI04X03.T01 one-dimensional and two-dimensional volumetric-flow-rate resultants at centers of cells in row 3
- AMI04X03.T01 one-dimensional and two-dimensional mass-flow-rate resultants at centers of cells in row 3.

Volumetric-flow-rate resultants at cell centers in row 3 are contained in the file AVI04X03.T01; an example is presented below.

Output records

Data item	Explanation							
1.	CR1,....,NR2———	50.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	1	0
1.	CR1,....,NR2———	150.00	10.00	.000000E+00	.886069E+01	.886069E+01	270.00	2	0
1.	CR1,....,NR2———	250.00	10.00	.000000E+00	.252433E+02	.252433E+02	270.00	3	0
1.	CR1,....,NR2———	350.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	4	0
1.	CR1,....,NR2———	450.00	10.00	.000000E+00	.252433E+02	.252433E+02	270.00	5	0
1.	CR1,....,NR2———	550.00	10.00	.000000E+00	.886069E+01	.886069E+01	270.00	6	0
1.	CR1,....,NR2———	650.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	7	0
1.	CR1,....,NR2———	50.00	-50.00	.177214E+00	.000000E+00	.177214E+00	.00	1	1
1.	CR1,....,NR2———	150.00	-50.00	.252438E+00	.885565E+01	.885925E+01	271.63	2	1
1.	CR1,....,NR2———	250.00	-50.00	.163831E+00	.256466E+02	.256471E+02	270.37	3	1
1.	CR1,....,NR2———	350.00	-50.00	.000000E+00	.000000E+00	.000000E+00	.00	4	1
1.	CR1,....,NR2———	450.00	-50.00	-.163840E+00	.256466E+02	.256471E+02	269.63	5	1
1.	CR1,....,NR2———	550.00	-50.00	-.252450E+00	.885565E+01	.885925E+01	268.37	6	1
1.	CR1,....,NR2———	650.00	-50.00	-.177219E+00	.000000E+00	.177219E+00	180.00	7	1
1.	CR1,....,NR2———	50.00	-150.00	.133109E+03	.000000E+00	.133109E+03	.00	1	2
1.	CR1,....,NR2———	150.00	-150.00	.197383E+03	-.122847E+01	.197387E+03	.36	2	2
1.	CR1,....,NR2———	250.00	-150.00	.494454E+03	-.489924E+01	.494478E+03	.57	3	2
1.	CR1,....,NR2———	350.00	-150.00	-.264146E+02	-.569723E+02	.627978E+02	114.87	4	2
1.	CR1,....,NR2———	450.00	-150.00	-.523984E+03	-.489924E+01	.524007E+03	179.46	5	2
1.	CR1,....,NR2———	550.00	-150.00	-.201282E+03	-.122847E+01	.201286E+03	179.65	6	2
1.	CR1,....,NR2———	650.00	-150.00	-.134676E+03	.000000E+00	.134676E+03	180.00	7	2
1.	CR1,....,NR2———	50.00	-250.00	.213488E+02	.000000E+00	.213488E+02	.00	1	3
1.	CR1,....,NR2———	150.00	-250.00	.228484E+02	-.113076E+02	.254933E+02	26.33	2	3
1.	CR1,....,NR2———	250.00	-250.00	.235404E+02	-.358484E+02	.428866E+02	56.71	3	3
1.	CR1,....,NR2———	350.00	-250.00	-.225954E-01	-.113945E+03	.113945E+03	90.01	4	3
1.	CR1,....,NR2———	450.00	-250.00	-.235889E+02	-.358484E+02	.429132E+02	123.35	5	3
1.	CR1,....,NR2———	550.00	-250.00	-.228941E+02	-.113076E+02	.255343E+02	153.71	6	3
1.	CR1,....,NR2———	650.00	-250.00	-.213885E+02	.000000E+00	.213885E+02	180.00	7	3

Column positions: 1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85

Mass-flow-rate resultants at cell centers in row 3 are contained in the file AMI04X03.T01; an example is presented below.

Output records

Data item | Explanation | 1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85

1.	CR1,....,NR2———	50.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	1	0
1.	CR1,....,NR2———	150.00	10.00	.000000E+00	.109832E-01	.109832E-01	270.00	2	0
1.	CR1,....,NR2———	250.00	10.00	.000000E+00	.312901E-01	.312901E-01	270.00	3	0
1.	CR1,....,NR2———	350.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	4	0
1.	CR1,....,NR2———	450.00	10.00	.000000E+00	.312901E-01	.312901E-01	270.00	5	0
1.	CR1,....,NR2———	550.00	10.00	.000000E+00	.109832E-01	.109832E-01	270.00	6	0
1.	CR1,....,NR2———	650.00	10.00	.000000E+00	.000000E+00	.000000E+00	.00	7	0
1.	CR1,....,NR2———	50.00	-50.00	.219664E-03	.000000E+00	.219664E-03	.00	1	1
1.	CR1,....,NR2———	150.00	-50.00	.312901E-03	.109768E-01	.109812E-01	271.63	2	1
1.	CR1,....,NR2———	250.00	-50.00	.203069E-03	.317886E-01	.317893E-01	270.37	3	1
1.	CR1,....,NR2———	350.00	-50.00	.000000E+00	.000000E+00	.000000E+00	.00	4	1
1.	CR1,....,NR2———	450.00	-50.00	-.203069E-03	.317886E-01	.317893E-01	269.63	5	1
1.	CR1,....,NR2———	550.00	-50.00	-.312901E-03	.109768E-01	.109812E-01	268.37	6	1
1.	CR1,....,NR2———	650.00	-50.00	-.219664E-03	.000000E+00	.219664E-03	180.00	7	1
1.	CR1,....,NR2———	50.00	-150.00	.164995E+00	.000000E+00	.164995E+00	.00	1	2
1.	CR1,....,NR2———	150.00	-150.00	.242779E+00	-.144141E-02	.242783E+00	.34	2	2
1.	CR1,....,NR2———	250.00	-150.00	.595405E+00	-.530501E-02	.595428E+00	.51	3	2
1.	CR1,....,NR2———	350.00	-150.00	.000000E+00	-.635576E-01	.635576E-01	90.00	4	2
1.	CR1,....,NR2———	450.00	-150.00	-.595405E+00	-.530501E-02	.595428E+00	179.49	5	2
1.	CR1,....,NR2———	550.00	-150.00	-.242779E+00	-.144141E-02	.242783E+00	179.66	6	2
1.	CR1,....,NR2———	650.00	-150.00	-.164995E+00	.000000E+00	.164995E+00	180.00	7	2
1.	CR1,....,NR2———	50.00	-250.00	.264627E-01	.000000E+00	.264627E-01	.00	1	3
1.	CR1,....,NR2———	150.00	-250.00	.282935E-01	-.138532E-01	.315029E-01	26.09	2	3
1.	CR1,....,NR2———	250.00	-250.00	.290953E-01	-.428971E-01	.518334E-01	55.85	3	3
1.	CR1,....,NR2———	350.00	-250.00	.000000E+00	-.127115E+00	.127115E+00	90.00	4	3
1.	CR1,....,NR2———	450.00	-250.00	-.290953E-01	-.428971E-01	.518334E-01	124.15	5	3
1.	CR1,....,NR2———	550.00	-250.00	-.282935E-01	-.138532E-01	.315029E-01	153.91	6	3
1.	CR1,....,NR2———	650.00	-250.00	-.264627E-01	.000000E+00	.264627E-01	180.00	7	3

Definition of Output Variables

The definitions of variables output to the two-dimensional parameter files are presented below. Variables are presented in the order in which they appear in the data file. Units in the output files correspond to original specifications.

CR1

- CR1 is the first of two spatial coordinates that define the point of application of the flow-rate resultants in a two-dimensional slice. Because the resultant flow rates are generated from orthogonal components whose lines of action intersect the centers of the cells, the resultants always act at the cell centers. CR1, therefore, represents the distance to the cell center from a specified origin. The location of the origin depends on the value of IV(36), which is specified in the POSTAIR input file INFILEx.POS. The value of IV(37) in INFILEx.POS does not affect CR1; however, the selection made for orientation of the output in INFILEx.POS, namely IV(39), affects CR1. If output is by layers or rows, CR1 will correspond to the distance along a row (in the X-direction). If output is by columns, CR1 will correspond to the distance along a column (in the Y-direction).
- CR1 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

CR2

- CR2 is the second of two spatial coordinates that define the point of application of the flow-rate resultants in a two-dimensional slice. Because the resultant flow rates are generated from orthogonal components whose lines of action intersect the centers of the cells, the resultants always act at the cell centers. CR2, therefore, represents the distance to the cell center from a specified origin. The location of the origin depends on the value of IV(36), which is specified in the POSTAIR input file INFILEx.POS. The value of IV(37) in INFILEx.POS does not affect CR2; however, the selection made for orientation of the output in INFILEx.POS, namely IV(39), affects CR2. If output is by layers, CR2 will correspond to the distance along a column (in the Y-direction). If output is by rows or columns, CR2 will correspond to a vertical elevation (in the Z-direction) generated from data contained in the MODEL.DAT file.
- CR2 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

FA1

- FA1 is the average flow rate in a particular direction acting at each cell center in a two-dimensional slice. FA1 is not generated directly by MODFLOW. Instead, MODFLOW calculates flow rates at cell faces. FA1 must be determined from the flow rates into and out of a cell in a particular direction. POSTAIR performs this operation by summing the component flow rates in the specified direction and then averaging them by dividing by two. FA1 can then be combined with a second average flow rate acting in an orthogonal direction to obtain a resultant two-dimensional flow rate which is applied at the center of the model cell (FR1). FA1 depends on the settings specified in the POSTAIR input file INFILEx.POS. In particular, FA1 depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers or rows, FA1 will correspond to the average flow rates along rows (in the X-direction). If output is by columns, FA1 will correspond to average flow rates along columns (in the Y-direction).

- FA1 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

FA2

- FA2 is the average flow rate in a direction perpendicular to FA1, acting at each cell center in a two-dimensional slice. FA2 is not generated directly by MODFLOW. Instead, MODFLOW calculates flow rates at cell faces. FA2 must then be determined from the flow rates into and out of a cell. POSTAIR performs this operation by summing the component flow rates in the orthogonal direction and then averaging them by dividing by two. FA2 can then be combined with FA1 to obtain a resultant two-dimensional flow rate which has its point of application at the center of the model cell (FR1). FA2 depends on the settings specified in the POSTAIR input file INFILEx.POS. In particular, FA2 depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers, FA2 will correspond to the average flow rates along columns (in the Y-direction). If output is by rows or columns, FA2 will correspond to average flow rates along layers (in the Z-direction).
- FA2 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

FR1

- FR1 is the magnitude of the resultant flow rates acting at the cell centers in a two-dimensional slice. FR1 is calculated by applying Pythagoras' Theorem to two orthogonal flow-rate components, FA1 and FA2, which are applied at the cell center, as follows: $FR1 = (FA1^2 + FA2^2)^{1/2}$. The determination of resultant flow rates is discussed in more detail in Section 4.3.7. Note that FR1 is a two-dimensional resultant. Output values thus depend on settings specified in the POSTAIR input file INFILEx.POS. In particular, FR1 depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers, FR1 will correspond to the resultant flow rates in the X-Y plane. If output is by rows, FR1 will correspond to resultant flow rates in the X-Z plane. If output is by columns, FR1 will correspond to resultant flow rates in the Y-Z plane.
- FR1 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

FD1

- FD1 is the direction in which the resultant flow rates act at the cell centers relative to the horizontal axis, in a two-dimensional slice. FD1 is calculated from two orthogonal flow rate components, FA1 and FA2, as follows: FD1 = arctan(FA1/FA2) radians, with FD1=0 along the horizontal axis. The resultant flow rates are discussed in more detail in Section 4.3.7. Note that FD1 is the direction of a two-dimensional resultant. Output values depend on settings specified in the POSTAIR input file INFILEx.POS. In particular, FD1 depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers or rows, FD1=0 along the X-axis. If output is by columns, FD1=0 along the Y-axis.

- FD1 is always present in the files that record resultant flow-rate output for two-dimensional slices in the model.

NR1

- NR1 is the first of two nodal coordinates that define the layer, row, or column number corresponding to the flow-rate resultants for a two-dimensional slice. The locations of the spatial- and nodal-coordinate origins are controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. NR1 also depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers or rows, NR1 will correspond to the column number. If output is by columns, NR1 will correspond to the row number.
- NR1 is always present in the files that record parameter output for two-dimensional slices in the model.

ND2

- ND2 is the second of two nodal coordinates that define the layer, row, or column number corresponding to the output parameter for a two-dimensional slice. The locations of the spatial- and nodal-coordinate origins are controlled by the variable IV(36) in the POSTAIR input file INFILEx.POS. ND2 also depends on the selection made for orientation of the output (variable IV(39) in INFILEx.POS). If output is by layers, ND2 will correspond to the row numbers. If output is by rows or columns, ND2 will correspond to the layer number.
- ND2 is always present in the files that record parameter output for two-dimensional slices in the model.

4.5.13 POSTAIR Resultant Flow Output Files for Each Cell

File Specification

Name of files:	One file for three-dimensional resultant volumetric flow rates per unit area at each cell and one file for three-dimensional resultant mass flow rates per unit area at each cell are generated (depending on the value of IV(41)) for the model domain. Each file is named directly by POSTAIR according to the convention described in Section 4.4.3.
File contents:	The files contain spatial coordinates, magnitudes of three-dimensional resultant flow rates per unit area, and nodal coordinates at each cell location in the model domain. For pneumatic simulations, flow rates for volumetric and mass flow per unit area are produced. For ground-water-flow simulations, only volumetric flow rates per unit area are produced.
File application:	These files record resultant volumetric- and mass-flow-rate-per-unit-area output generated by POSTAIR from three orthogonal components at each cell.

Program output:	Output to the head/pressure and flow files is accomplished in the subroutine R3FLOW.
Physical units:	Unit systems for length, volume, time, pressure, temperature, mass, and permeability input and output are specified by the user when data are entered into the preprocessor. Output units correspond to initial settings. If no unit system was specified, output units conform to the default unit systems for each parameter.

File Structure

The structure of the three-dimensional flow-per-unit-area files for each cell in the model domain is as follows. Item 1 is output (NROW)(NCOL)(NLAY) times and is oriented by layers.

1. Data: CX,CY,CZ,FR3,NC,NR,NL
   Format: 3F15.5,E20.8,3I5)

Output-file names are generated directly by POSTAIR according to the convention described in Section 4.4.3.

Example Output File

Values specified in the POSTAIR input file INFILEx.POS control the nature and extent of the simulation output. For example, the values specified in the input file listed in Section 4.5.3 require that:

- pressure and flow output (IV(38)=2) be generated for the air-flow simulation (IV(35)=2)
- output is by layers regardless of IV(39) setting and generated for every cell regardless of IV(43) setting
- spatial and nodal coordinates conform with MODFLOW convention (IV(36)=1)
- three-dimensional flow-rate resultants are generated (IV(41)=4) and spatial coordinates for flow rates at cell faces reflect cell faces (IV(37)=1)
- simulation identification number is 4 (IV(40)=04).

With the above settings in the data file given in Section 4.5.3, the following three-dimensional resultant-flow-rate-per-unit-area output files are generated for time step 1 (T01) and simulation number 4 (04):

- 3DQRV04.T01 three-dimensional volumetric-flow-rate resultants per unit area at the center of each cell in model domain
- 3DQRM04.T01 three-dimensional mass-flow-rate resultants per unit area at the center of each cell in model domain.

Three-dimensional volumetric-flow-rate resultants per unit area at cell centers in layers 0 through 3 are contained in the file 3DQRV04.T01; selected output from this file is presented below.

Output records

Data item	Explanation	1–10	11–20	21–30	31–45	46–50	51–55	56–60
1.	CX,......,NL	50.00000	50.00000	-50.00000	0.00000000E+00	1	1	1
1.	CX,......,NL	150.00000	50.00000	-50.00000	0.15157619E-04	2	1	1
1.	CX,......,NL	250.00000	50.00000	-50.00000	0.37695005E-04	3	1	1
1.	CX,......,NL	350.00000	50.00000	-50.00000	0.65236047E-04	4	1	1
1.	CX,......,NL	450.00000	50.00000	-50.00000	0.37695005E-04	5	1	1
1.	CX,......,NL	550.00000	50.00000	-50.00000	0.15157619E-04	6	1	1
1.	CX,......,NL	650.00000	50.00000	-50.00000	0.00000000E+00	7	1	1
1.	CX,......,NL	50.00000	150.00000	-50.00000	0.15157619E-04	1	2	1
1.	CX,......,NL	150.00000	150.00000	-50.00000	0.53469162E-03	2	2	1
1.	CX,......,NL	250.00000	150.00000	-50.00000	0.13324182E-02	3	2	1
1.	CX,......,NL	350.00000	150.00000	-50.00000	0.23917910E-02	4	2	1
1.	CX,......,NL	450.00000	150.00000	-50.00000	0.13323711E-02	5	2	1
1.	CX,......,NL	550.00000	150.00000	-50.00000	0.53456152E-03	6	2	1
1.	CX,......,NL	650.00000	150.00000	-50.00000	0.10718055E-04	7	2	1
1.	CX,......,NL	50.00000	250.00000	-50.00000	0.25063087E-04	1	3	1
1.	CX,......,NL	150.00000	250.00000	-50.00000	0.88573899E-03	2	3	1
1.	CX,......,NL	250.00000	250.00000	-50.00000	0.26052298E-02	3	3	1
1.	CX,......,NL	350.00000	250.00000	-50.00000	0.00000000E+00	4	3	1
1.	CX,......,NL	450.00000	250.00000	-50.00000	0.26054359E-02	5	3	1
1.	CX,......,NL	550.00000	250.00000	-50.00000	0.88531006E-03	6	3	1
1.	CX,......,NL	650.00000	250.00000	-50.00000	0.17722279E-04	7	3	1
1.	CX,......,NL	50.00000	350.00000	-50.00000	0.15157619E-04	1	4	1
1.	CX,......,NL	150.00000	350.00000	-50.00000	0.53475320E-03	2	4	1
1.	CX,......,NL	250.00000	350.00000	-50.00000	0.13324716E-02	3	4	1
1.	CX,......,NL	350.00000	350.00000	-50.00000	0.23922359E-02	4	4	1
1.	CX,......,NL	450.00000	350.00000	-50.00000	0.13324246E-02	5	4	1
1.	CX,......,NL	550.00000	350.00000	-50.00000	0.53462310E-03	6	4	1
1.	CX,......,NL	650.00000	350.00000	-50.00000	0.10718055E-04	7	4	1

Output records

Data item	Explanation	1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80						
1.	CX,.......,NL———	50.00000	450.00000	-50.00000	0.00000000E+00	1	5	1
1.	CX,.......,NL———	150.00000	450.00000	-50.00000	0.10718055E-04	2	5	1
1.	CX,.......,NL———	250.00000	450.00000	-50.00000	0.26654392E-04	3	5	1
1.	CX,.......,NL———	350.00000	450.00000	-50.00000	0.46128851E-04	4	5	1
1.	CX,.......,NL———	450.00000	450.00000	-50.00000	0.26654392E-04	5	5	1
1.	CX,.......,NL———	550.00000	450.00000	-50.00000	0.10718055E-04	6	5	1
1.	CX,.......,NL———	650.00000	450.00000	-50.00000	0.00000000E+00	7	5	1

Three-dimensional mass-flow-rate resultants per unit area at cell centers in layers 0 through 3, are contained in the file 3DQRM04.T01; selected output from this file is presented below.

Output records

Data item	Explanation	1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80						
1.	CX,.......,NL———	50.00000	50.00000	-50.00000	0.00000000E+00	1	1	1
1.	CX,.......,NL———	150.00000	50.00000	-50.00000	0.18789425E-07	2	1	1
1.	CX,.......,NL———	250.00000	50.00000	-50.00000	0.46726829E-07	3	1	1
1.	CX,.......,NL———	350.00000	50.00000	-50.00000	0.80866783E-07	4	1	1
1.	CX,.......,NL———	450.00000	50.00000	-50.00000	0.46726829E-07	5	1	1
1.	CX,.......,NL———	550.00000	50.00000	-50.00000	0.18789425E-07	6	1	1
1.	CX,.......,NL———	650.00000	50.00000	-50.00000	0.00000000E+00	7	1	1
1.	CX,.......,NL———	50.00000	150.00000	-50.00000	0.18789425E-07	1	2	1
1.	CX,.......,NL———	150.00000	150.00000	-50.00000	0.66279284E-06	2	2	1
1.	CX,.......,NL———	250.00000	150.00000	-50.00000	0.16515928E-05	3	2	1
1.	CX,.......,NL———	350.00000	150.00000	-50.00000	0.29646330E-05	4	2	1
1.	CX,.......,NL———	450.00000	150.00000	-50.00000	0.16515345E-05	5	2	1
1.	CX,.......,NL———	550.00000	150.00000	-50.00000	0.66263163E-06	6	2	1
1.	CX,.......,NL———	650.00000	150.00000	-50.00000	0.13286130E-07	7	2	1
1.	CX,.......,NL———	50.00000	250.00000	-50.00000	0.31068268E-07	1	3	1
1.	CX,.......,NL———	150.00000	250.00000	-50.00000	0.10979306E-05	2	3	1

Output records

Data item	Explanation	1 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80						
1.	CX,.......,NL———	250.00000	250.00000	-50.00000	0.32291666E-05	3	3	1
1.	CX,.......,NL———	350.00000	250.00000	-50.00000	0.00000000E+00	4	3	1
1.	CX,.......,NL———	450.00000	250.00000	-50.00000	0.32294220E-05	5	3	1
1.	CX,.......,NL———	550.00000	250.00000	-50.00000	0.10973990E-05	6	3	1
1.	CX,.......,NL———	650.00000	250.00000	-50.00000	0.21968583E-07	7	3	1
1.	CX,.......,NL———	50.00000	350.00000	-50.00000	0.18789425E-07	1	4	1
1.	CX,.......,NL———	150.00000	350.00000	-50.00000	0.66286913E-06	2	4	1
1.	CX,.......,NL———	250.00000	350.00000	-50.00000	0.16516591E-05	3	4	1
1.	CX,.......,NL———	350.00000	350.00000	-50.00000	0.29651844E-05	4	4	1
1.	CX,.......,NL———	450.00000	350.00000	-50.00000	0.16516008E-05	5	4	1
1.	CX,.......,NL———	550.00000	350.00000	-50.00000	0.66270792E-06	6	4	1
1.	CX,.......,NL———	650.00000	350.00000	-50.00000	0.13286130E-07	7	4	1
1.	CX,.......,NL———	50.00000	450.00000	-50.00000	0.00000000E+00	1	5	1
1.	CX,.......,NL———	150.00000	450.00000	-50.00000	0.13286130E-07	2	5	1
1.	CX,.......,NL———	250.00000	450.00000	-50.00000	0.33040855E-07	3	5	1
1.	CX,.......,NL———	350.00000	450.00000	-50.00000	0.57181449E-07	4	5	1
1.	CX,.......,NL———	450.00000	450.00000	-50.00000	0.33040855E-07	5	5	1
1.	CX,.......,NL———	550.00000	450.00000	-50.00000	0.13286130E-07	6	5	1
1.	CX,.......,NL———	650.00000	450.00000	-50.00000	0.00000000E+00	7	5	1

Definition of Output Variables

The definitions of variables output to the two-dimensional parameter files are presented below. Variables are presented in the order in which they appear in the data file. Units in the output files correspond to original specifications.

CX

- CX is the first of three spatial coordinates that define the point of application of the three-dimensional flow-rate resultants per unit area at each cell in the model domain. Note that, although the resultant flow rates per unit area are generated from orthogonal components that act at the cell faces, the value of CX represents the distance from the origin to the cell center in the X-direction. The location of the origin depends on the value of IV(36), which is specified in the POSTAIR input file INFILEx.POS.
- CX is always present in the files that record three-dimensional resultant flow-rate output for each cell in the model.

CY

- CY is the second of three spatial coordinates that define the point of application of the three-dimensional flow-rate resultants per unit area at each cell in the model domain. Note that, although the resultant flow rates per unit area are generated from orthogonal components that act at the cell faces, the value of CY represents the distance from the origin to the cell center in the Y-direction. The location of the origin depends on the value of IV(36), which is specified in the POSTAIR input file INFILEx.POS.
- CY is always present in the files that record three-dimensional resultant flow-rate output for each cell in the model.

CZ

- CZ is the third of three spatial coordinates that define the point of application of the three-dimensional flow-rate resultants per unit area at each cell in the model domain. Note that, although the resultant flow rates per unit area are generated from orthogonal components that act at the cell faces, the value of CZ represents the distance from the origin to the cell center in the Z-direction. The location of the origin depends on the value of IV(36), which is specified in the POSTAIR input file INFILEx.POS.
- CZ is always present in the files that record three-dimensional resultant flow-rate output for each cell in the model.

F3

- F3 is the magnitude of the three-dimensional resultant flow rate per unit area acting at each cell in the model domain. F3 is calculated by applying Pythagoras' Theorem to three orthogonal flow-rate components (Fx, Fy, Fz) which are divided by the area of the cell face through which they act (Ax, Ay, Az) as follows: $F3 = ((Fx/Ax)^2 + (Fy/Ay)^2 + (Fz/Az)^2)^{1/2}$. The determination of resultant flow rates is discussed in more detail in Section 4.3.7.
- F3 is always present in the files that record three-dimensional resultant flow rates per unit area for each cell in the model.

NR

- NR is the first of three nodal coordinates that define the layer, row, and column number corresponding to the three-dimensional resultant flow rates per unit area for each cell in the model.
- NR is always present in the files that record parameters output for three-dimensional resultant flows per unit area at each model cell.

NC

- NC is the second of three nodal coordinates that define the layer, row, and column number corresponding to the three-dimensional resultant flow rates per unit area for each cell in the model.
- NC is always present in the files that record parameters output for three-dimensional resultant flows per unit area at each model cell.

NL

- NL is the third of three nodal coordinates that define the layer, row, and column number corresponding to the three-dimensional resultant flow rates per unit area for each cell in the model.
- NL is always present in the files that record parameters output for three-dimensional resultant flows per unit area at each model cell.

4.5.14 POSTAIR Mass Balance and Well Output File

File Specification

Name of file:	One file is generated for each time step during the air-flow simulation and named directly by POSTAIR according to the convention described in Section 4.4. (for example, MASSxx.Txx).
File contents:	Mass flow rates through atmospheric layer, left side of domain, back side of domain, right side of domain, front side of domain, and wells/trenches; total mass flow across model boundaries; relative and absolute mass balances; percent recharge from atmosphere and percent recharge from lateral boundaries; mass flow, volumetric flow, and pressures in individual wells and trenches; unit summary for air-flow simulation. Output is generated only if IV(42)=1 and IV(38)=2 is specified in the POSTAIR input file INFILEx.POS.
File application:	This file records mass-balance and well/trench output generated by POSTAIR at the end of each time step and unit summaries for air-flow simulations.
Fortran unit number:	The program defines the output file as UNIT = 24.
Program output:	Output is controlled in the subroutine AFLOW. Output is written directly to the file.
Physical units:	Units for mass flow rates, volumetric flow rates, and well/trench pressures conform to those specified by the user when the data are entered into the preprocessor. If no unit system is specified, output units will conform to the default unit systems for each parameter.

File Structure

The structure of the mass-balance/well output file is as follows:

Output items 1 through 10 once for each time step.

1. Data: AMASSA
   Format: E12.4

2. Data: AMASSL
   Format: E12.4

3. Data: AMASSB
   Format: E12.4

4. Data: AMASSR
   Format: E12.4

5. Data: AMASSF
   Format: E12.4

6. Data: AMTR
   Format: E12.4

7. Data: AMASSW
   Format: E12.4

8. Data: AMMBA
   Format: E12.4

9. Data: AMPAR
   Format: F10.2

10. Data: AMPRL
    Format: F10.2

11. Data: AMYY
    Format: F10.2

Output items 12 through 14 once for each well and trench.

12. Data: WELLQM(IW,1)
    Format: E12.4

13. Data: WELLQM(IW,3)
    Format: E12.4

14. Data: WELLQM(IW,2)
    Format: E12.4

Example Output File

Values specified in the POSTAIR input file INFILEx.POS control the nature and extent of the simulation output. For example, the values specified in the input file listed in Section 4.5.3 require that:

- pressure and flow output (IV(38)=2) be generated for the air-flow simulation (IV(35)=2)
- output be oriented by rows (IV(39)=2) and generated for a single two-dimensional slice (row 3, IV(43)=3)
- spatial and nodal coordinates conform with MODFLOW convention (IV(36)=1)
- a mass balance be performed (IV(42)=1)
- the simulation identification number is 4 (IV(40)=04)

For the values given in Section 4.5.3, the mass-balance/well output file MASS04.T01 given below is generated for time step 1 and simulation number 4.

```
          MASS BALANCE / WELL / UNIT OUTPUT FOR SIMULATION # 01
          ==== =======   ====   ==== ====== === ========== = ==

     MASS FLOW INTO DOMAIN IS POSITIVE

     MASS FLOW OUT OF DOMAIN IS NEGATIVE

MASS BALANCE OUTPUT FOR TIME STEP :  1

MASS FLOW RATE THROUGH MODEL ATMOSPHERIC LAYER       :   .2344E+00  g/s

MASS FLOW RATE THROUGH LEFT SIDE OF MODEL DOMAIN     :   .4266E+00  g/s

MASS FLOW RATE THROUGH BACK SIDE OF MODEL DOMAIN     :   .1300E+01  g/s

MASS FLOW RATE THROUGH RIGHT SIDE OF MODEL DOMAIN    :   .4266E+00  g/s

MASS FLOW RATE THROUGH FRONT SIDE OF MODEL DOMAIN    :   .1300E+01  g/s


TOTAL MASS FLOW RATE ACROSS MODEL BOUNDARIES         :   .3688E+01  g/s

TOTAL MASS FLOW RATE THROUGH WELLS / TRENCHES        :  -.3688E+01  g/s

FLOW ACROSS BOUNDARIES - FLOW THROUGH WELLS/TRENCHES :   .2384E-06  g/s


PERCENT AIR RECHARGE FROM ATMOSPHERE                 :      6.40 percent

PERCENT AIR RECHARGE FROM LATERAL BOUNDARIES         :     93.60 percent

NORMALIZED MASS BALANCE (FLOW IN-FLOW OUT)/TOTAL FLOW :     0.00 percent

MASS FLOW RATES THROUGH WELLS/TRENCHES FOR TIME STEP  :  1

MASS FLOW RATE THROUGH WELL NUMBER     1             :  -.3688E+01  g/s

VOLUMETRIC FLOW RATES THROUGH WELLS/TRENCHES FOR TIME STEP :  1

VOLUMETRIC FLOW RATE THROUGH WELL NUMBER     1       :  -.3306E+04 cm^3/s

PRESSURE IN WELLS / TRENCHES FOR TIME STEP :  1

PRESSURE IN WELL NUMBER    1                         :   .9000E+00 atm
```

```
SUMMARY OF UNITS USED IN SIMULATION

LENGTH UNIT SYSTEM      :  cm

VOLUME UNIT SYSTEM      :  cm^3

TIME UNIT SYSTEM        :  s

PRESSURE UNIT SYSTEM    :  atm

TEMPERATURE UNIT SYSTEM :  degC

MASS UNIT SYSTEM        :   g

PERMEABILITY UNIT SYSTEM:  cm^2
```

Definition of Output Variables

The definitions of mass-balance and well terms output to the MASSxx.Txx file are presented below. Variables are presented in the order in which they appear in the data file. Units in the output files correspond to original specifications.

AMASSA

- AMASSA is the mass flow rate through the superimposed atmospheric layer. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSA is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in the atmospheric layer.
- AMASSA is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMASSL

- AMASSL is the mass flow rate through the left side of the model domain. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSL is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in column 1 (layers 2 through NLAY).
- AMASSL is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMASSB

- AMASSB is the mass flow rate through the back side of the model domain. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSB is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in row 1 (layers 2 through NLAY).
- AMASSB is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMASSR

- AMASSR is the mass flow rate through the right side of the model domain. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSR is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in column NCOL (layers 2 through NLAY).
- AMASSR is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMASSF

- AMASSF is the mass flow rate through the front side of the model domain. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSF is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in row NROW (layers 2 through NLAY).
- AMASSF is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMTR

- AMTR is the total mass flow rate across the exterior model boundaries. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMTR is calculated in POSTAIR by summing the mass flow rates at each constant-head cell in the superimposed atmospheric layer (layer zero) and at each constant-head cell in the lateral boundary.
- AMTR is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMASSW

- AMASSW is the total mass flow rate through the individual wells/trenches in the model domain. Mass flow into the model domain is positive and mass flow out of the model domain is negative. AMASSW is calculated in POSTAIR by summing the mass flow rates at constant-head cells defining the wells or trenches in the interior of the model domain.
- AMASSW is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMMBA

- AMMBA is the absolute mass balance for the simulation time step. AMMBA is calculated as the difference between the air-flow rates into the model domain and the air-flow rates out of the model domain. The sign convention used for the flow rates is that air-flow into the model domain is positive and air flow out of the model domain is negative. AMMBA is calculated in POSTAIR as follows:

$$AMMBA = AMASSA + AMASSL + AMASSB + AMASSR + AMASSF + \Sigma\ (AMASSW).$$

- AMMBA is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMMBR

- AMMBR is the relative mass balance for the simulation time step:

$$AMMBR = \frac{(\text{Mass Rate In} - \text{Mass Rate Out})}{(ABS(\text{Mass Rate In}) + ABS(\text{Mass Rate Out})) / 2.0} \times 100$$

- AMMBR is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMPAR

- AMPAR is the percentage recharge (or loss) of air into (or out of) the model domain through the atmospheric layer. In theory, AMPAR approaches 100 percent. AMPAR can be increased by extending lateral boundaries or increasing vertical permeabilities of confining units. AMPAR is calculated in POSTAIR as follows: AMPAR=(AMASSA)/(AMASSA+AMASSL+AMASSB+ AMASSR+AMASSF)*100.
- AMPAR is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

AMPRL

- AMPRL is the percentage recharge (or loss) of air into (or out of) the model domain through the lateral boundaries. In theory, AMPRL approaches 0 percent. AMPRL can be reduced by extending lateral boundaries or increasing vertical permeabilities of confining units. AMPRL is calculated in POSTAIR as follows: AMPRL=100-AMPAR.
- AMPRL is always present in the MASSxx.Txx file, which is generated by setting IV(42)=1 and IV(38)=2 in the POSTAIR input file INFILEx.POS.

SECTION 5.0--AIR3D MODEL TESTING

5.1 Analytical Solutions

The computer codes collectively referred to as AIR3D presented in this report implement a numerical solution to the generalized, three-dimensional air-flow equation. As a method of testing the package, pressure and flow output were compared to analytical solutions.

5.1.1 Model Testing with Analytical Solutions

The analytical solutions used for model testing are for steady, two- dimensional, axisymmetric air flow to a well and are reported by Baehr and Joss (in press). Two cases were investigated--

- domain connected directly to the atmosphere
- domain separated from the atmosphere by a confining unit.

5.1.2 Air-flow Model for a Domain Connected Directly to the Atmosphere

The simulated domain is shown in figure 9. The top of the unsaturated zone is assumed to be directly connected to the atmosphere. The bottom boundary is formed by the water table or an impervious unit. The analytical solution from Baehr and Joss (in press) is as follows:

$$\phi = P_{atm}^2 + \frac{2aQ^*}{\pi^2 k_r (l-d) r_w} \tag{34}$$

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

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 $(k_r/k_z)^{½}$	[-]
r_w	= radius of the well (to filter/soil interface)	[cm]
r	= radial distance from well center line	[cm]
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 (34) is the solution to the steady-state air-flow equation for a radially symmetric domain connected directly to the atmosphere. Equation (34) can be used to determine pressure distribution in the domain.

By differentiating equation (34) with respect to the two principal directions (r and z), pressure gradients are obtained that can be used to determine horizontal and vertical components of specific discharge as follows:

$$\frac{\partial \phi}{\partial r} = \frac{-K}{a}\left\{\sum_{n=1}^{\infty} M_m\, \alpha_m \sin(M_m z)\, K_1\!\left(M_m \frac{r}{a}\right)\right\} \qquad (35)$$

$$\frac{\partial \phi}{\partial z} = \frac{\pi K}{b}\left\{\sum_{n=1}^{\infty} m\, \alpha_m \cos(M_m z)\, K_0\!\left(M_m \frac{r}{a}\right)\right\} \qquad (36)$$

where

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

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

Volumetric specific discharge in the horizontal (r) and vertical (z) directions are given by:

$$q_{rv} = -\frac{k_r}{2\,\mu\,\sqrt{\phi}}\,\frac{\partial\phi}{\partial r} \qquad (37)$$

$$q_{zv} = -\frac{k_z}{2\,\mu\,\sqrt{\phi}}\,\frac{\partial\phi}{\partial z} \qquad (38)$$

where

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

Mass specific discharge in the horizontal and vertical directions are given by:

$$q_{rm} = -\frac{\omega\,k_r}{2\,\mu\,R\,T}\,\frac{\partial\phi}{\partial r} \qquad (39)$$

$$q_{zm} = -\frac{\omega\,k_z}{2\,\mu\,R\,T}\,\frac{\partial\phi}{\partial z} \qquad (40)$$

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 (35) and $(\partial\phi/\partial z)$ is given by equation (36).

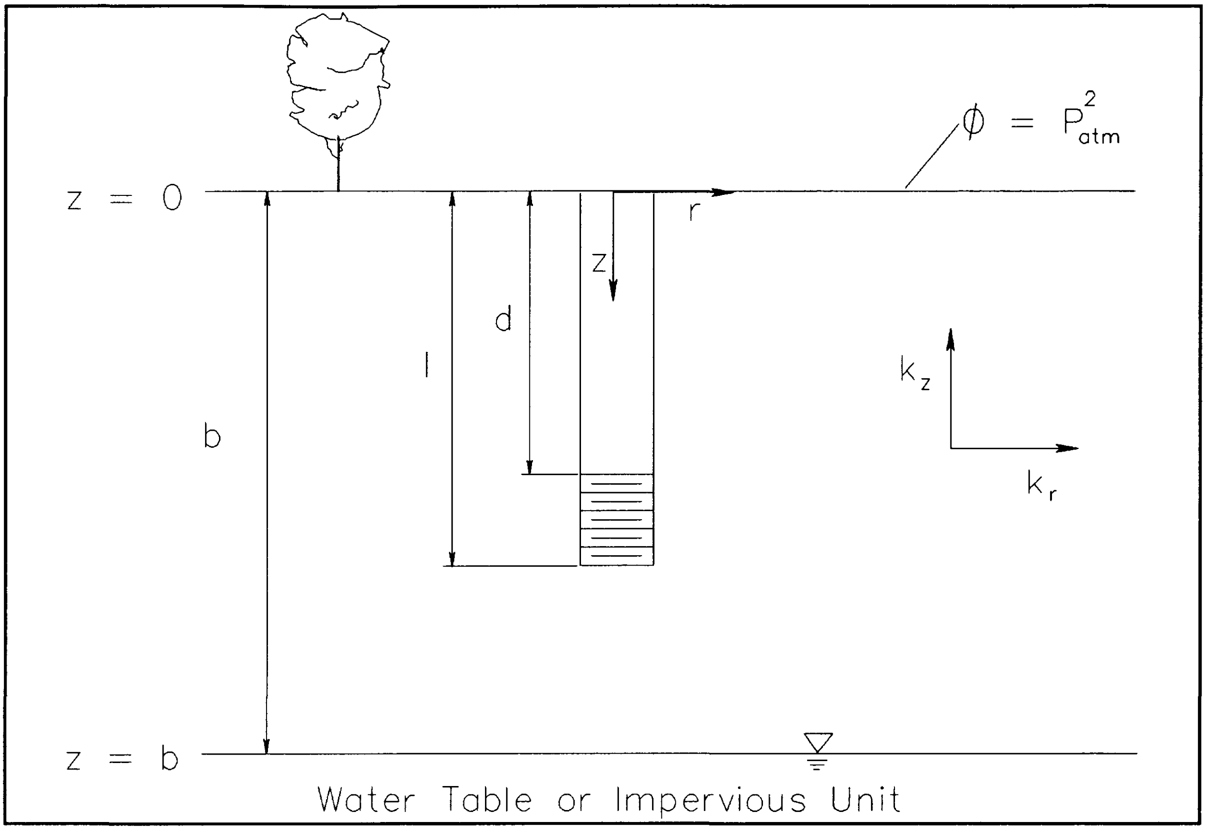

Figure 9.--Domain connected directly to land surface.

5.1.3 Air-flow Model for a Domain Separated From the Atmosphere by a Confining Unit

The simulated domain is shown in Figure 10. The upper leaky unit can be, for example, a stratum less permeable to air than the domain or, perhaps, a slightly permeable paved surface. The bottom boundary is the water table or an impervious unit. This solution models the confining unit directly by using the generalized cosine transformation. The analytical solution from Baehr and Joss (in press) is as follows:

$$\phi = P_{atm}^2 + \frac{2 h Q^* a b}{\pi k_r (l-d) r_w} \tag{41}$$

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

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]

q_n is determined numerically by the Newton Rhapson algorithm, from an initial estimate:

$$q_n^{(0)} = \pi(n - \frac{3}{4})$$

Equation (41) is the solution to the steady-state air-flow equation for a radially symmetric domain separated from the atmosphere by a confining unit. By differentiating equation (41) with respect to the two principal directions (r and z), pressure gradients are obtained that can be used to determine horizontal and vertical components of specific discharge.

Pressure gradients for the general model are given by:

$$\frac{\partial\phi}{\partial r} = -\frac{K}{ab}\left\{\sum_{n=1}^{\infty} q_n \alpha_n \cos\left(q_n\left(\frac{b-z}{b}\right)\right) K_1\left(\frac{q_n r}{a\,b}\right)\right\} \quad (42)$$

and

$$\frac{\partial\phi}{\partial z} = -\frac{K}{b}\left\{\sum_{n=1}^{\infty} q_n \alpha_n \sin\left(q_n\left(\frac{b-z}{b}\right)\right) K_0\left(\frac{q_n r}{a\,b}\right)\right\} \quad (43)$$

where

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

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

Volumetric specific discharge in the horizontal (r) and vertical (z) directions can be determined by substituting the above expressions for $(\partial\phi/\partial r)$ and $(\partial\phi/\partial z)$ into equations (37) and (38), respectively. Similarly, the mass specific discharge in the horizontal and vertical directions can be determined by substituting the above expressions for $(\partial\phi/\partial r)$ and $(\partial\phi/\partial z)$ into equations (39) and (40), respectively.

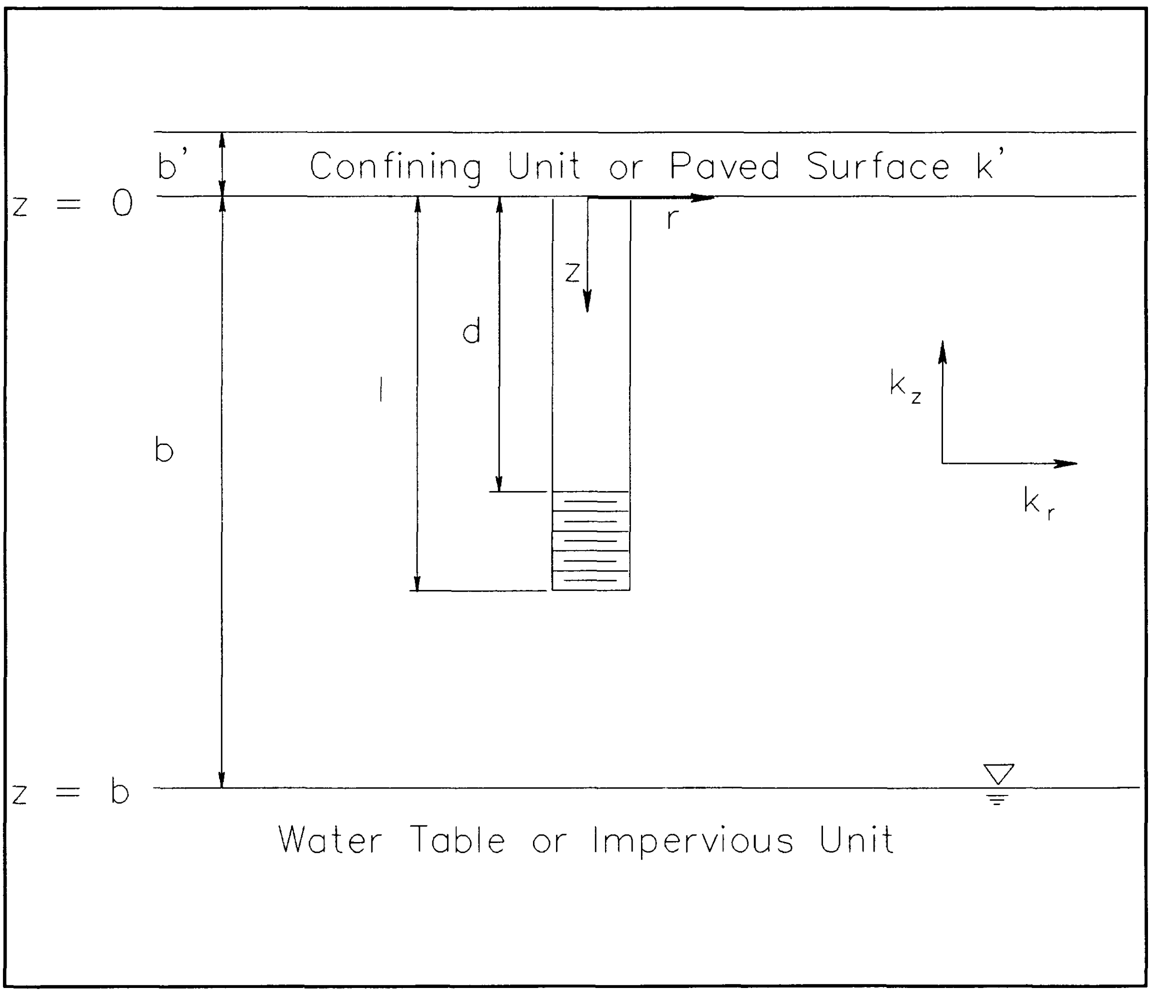

Figure 10.--Domain separated from the atmosphere by a leaky confining unit.

5.2 Model Testing For a Domain Open to the Atmosphere

5.2.1 Model for a Domain Open to the Atmosphere

To test the numerical solution implemented by AIR3D to the analytical solution given by equation (35), flow to a single extraction well in a homogeneous, anisotropic ($k_x \neq k_z$) domain was simulated with the following parameter specifications (refer to fig. 9):

- length d = 100 cm
- length l = 160 cm
- depth b = 260 cm
- radius r_w = 10.0 cm .

The following air-phase permeabilities k_x, k_y, and k_z are assigned:

- air permeability in X-direction = 1.000E-08 cm^2
- air permeability in Y-direction = 1.000E-08 cm^2
- air permeability in Z-direction = 2.000E-08 cm^2.

A steady-state simulation was performed by assuming a well pressure of 0.90 atm for the numerical solution; this corresponds to a mass withdrawal rate of Q=1.209 g/s for input to the analytical solution.

5.2.2 Input File

The data input file (DATAIRx.PRE) for the numerical air-flow model is as follows:

```
3 DIMENSIONAL AIR FLOW ANALYSIS (DOMAIN OPEN TO ATMOSPHERE)
13 LAYERS, 41 ROWS, 41 COLUMNS
    1    1    1    1    1    1    1
         13        41        41         1
          1         1         0
          1
       1.00
    1   21   21   21   21    6    8     0.900
    3600.00         1       1.0
          1
     3020.0       1(6F10.1)
      160.0     160.0     160.0     160.0     160.0      80.0
       80.0      80.0      80.0      80.0      40.0      40.0
       40.0      40.0      40.0      20.0      20.0      20.0
       20.0      20.0      20.0      20.0      20.0      20.0
```

```
    20.0      20.0      40.0      40.0      40.0      40.0
    40.0      80.0      80.0      80.0      80.0      80.0
   160.0     160.0     160.0     160.0     160.0
  3020.0         1(6F10.1)
   160.0     160.0     160.0     160.0     160.0      80.0
    80.0      80.0      80.0      80.0      40.0      40.0
    40.0      40.0      40.0      20.0      20.0      20.0
    20.0      20.0      20.0      20.0      20.0      20.0
    20.0      20.0      40.0      40.0      40.0      40.0
    40.0      80.0      80.0      80.0      80.0      80.0
   160.0     160.0     160.0     160.0     160.0

       1     260.0
       1        13     260.0 1.000E-08   1.0 2.000E-08 0.30
```

5.2.3 Mass Balance for Numerical Simulation

The following results of the numerical simulation summarize mass flow rates for air entering and exiting the model domain:

Mass Balance / Well / Unit Output For Domain Open To Atmosphere

Mass flow into domain is positive
Mass flow out of domain is negative

Mass balance output for time step : 1	
Mass flow rate through model atmospheric layer	: 0.1145e+01 g/sec
Mass flow rate through left side of model domain	: 0.5994e-05 g/sec
Mass flow rate through back side of model domain	: 0.5994e-05 g/sec
Mass flow rate through right side of model domain	: 0.5994e-05 g/sec
Mass flow rate through front side of model domain	: 0.5994e-05 g/sec
Total mass flow rate across model boundaries	: 0.1145e+01 g/sec
Total mass flow rate through wells / trenches	: -0.1145e+01 g/sec
Flow across boundaries - flow through wells/trenches	: -0.1298e-05 g/sec
Percent air recharge from atmosphere	: 100.00 %
Percent air recharge from lateral boundaries	: 0.00 %
Normalized mass balance (flow in-flow out)/total flow	: 0.00 %
Mass flow rates through wells/trenches for time step : 1	
Mass flow rate through well number 1	: -0.1145e+01 g/sec

Volumetric flow rates through wells/trenches for time step : 1
Volumetric flow rate through well number 1 : -0.1027e+04 cm^3/sec
Pressure in wells / trenches for time step : 1
Pressure in well number 1 : 0.9000e+00 atm

5.2.4 Comparison of analytical and numerical solutions

The mass flow rate out of the well (1.145 g/s) was used as input to the analytical model. Model predictions from the analytical solution were compared with the numerical predictions for pneumatic pressure, horizontal air-flow rates, and vertical air-flow rates at 50 centimeters below grade. Flow output was normalized to specific discharge for the numerical solution by dividing by the area of a face.

The pressure comparison between the analytical and numerical solutions is illustrated in figure 11. The horizontal component of mass flow for the numerical and analytical solutions is illustrated in figure 12. The vertical component of mass flow for the numerical and analytical solutions is illustrated in figure 13. The fit illustrated in figures 11 through 13 indicates that the numerical solution was implemented properly.

5.3 Model Testing For a Domain Separated from the Atmosphere by a Confining Unit

5.3.1 Model for a Domain Separated from the Atmosphere by a Confining Unit

Model Configuration

To test the numerical solution implemented by AIR3D to the analytical solution given by equation (41), the parameters are specified as follows (refer to fig. 10):

- length d = 100 cm
- length l = 160 cm
- depth b = 260 cm
- radius r_w = 10.0 cm
- confining-unit thickness b' = 20 cm .

The following air-phase permeabilities are assigned:

- air permeability in X-direction = 1.000E-08 cm^2
- air permeability in Y-direction = 1.000E-08 cm^2
- air permeability in Z-direction = 2.000E-08 cm^2
- air permeability of confining unit = 1.000E-10 cm^2 .

A steady-state simulation was performed by using an assumed well pressure of 0.90 atm, which corresponds to a mass withdrawal rate Q=0.974 g/s for input to the analytical solution.

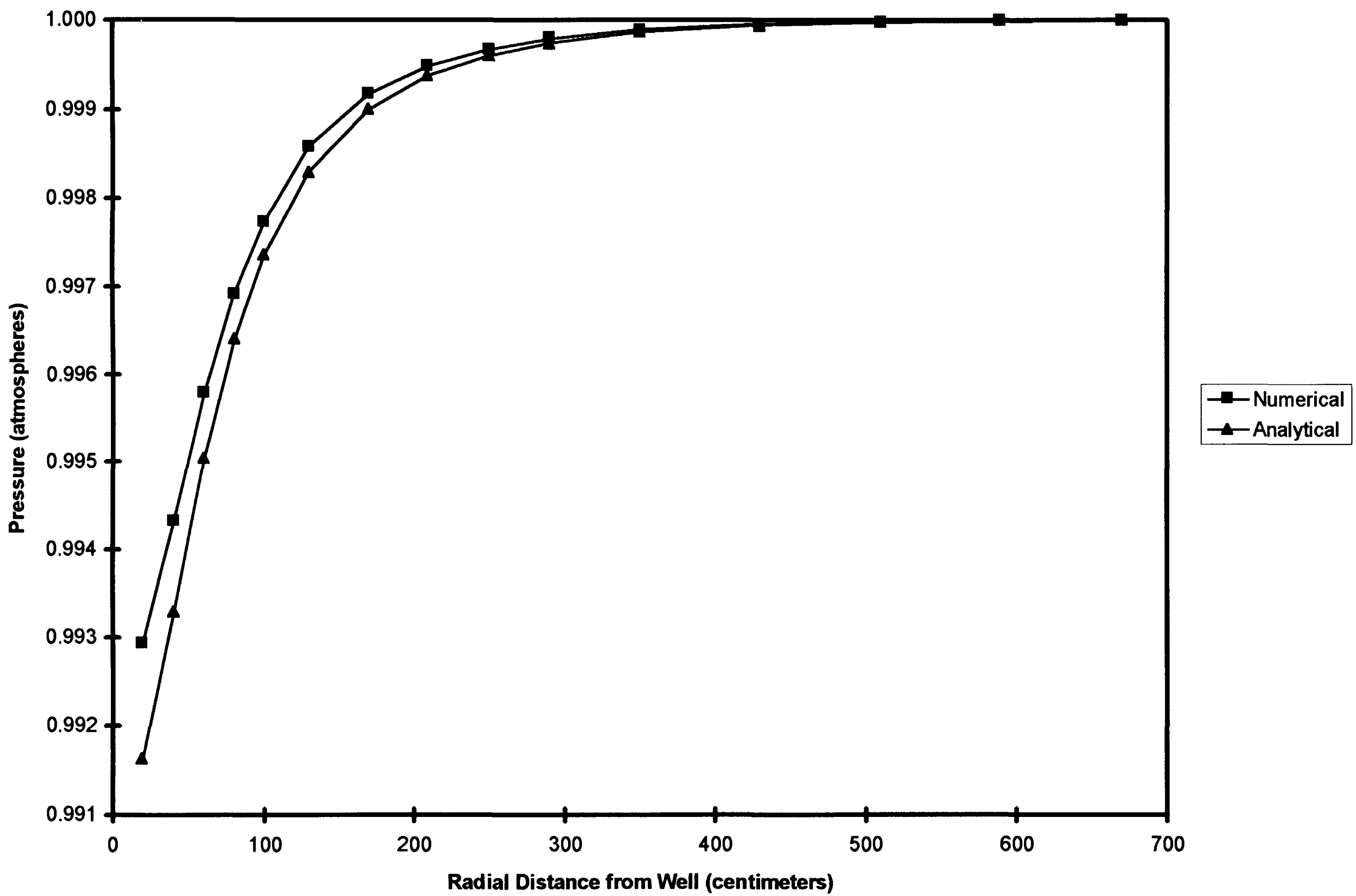

Figure 11.--Numerical and analytical pressure predictions at 50 centimeters below grade for domain open to atmosphere.

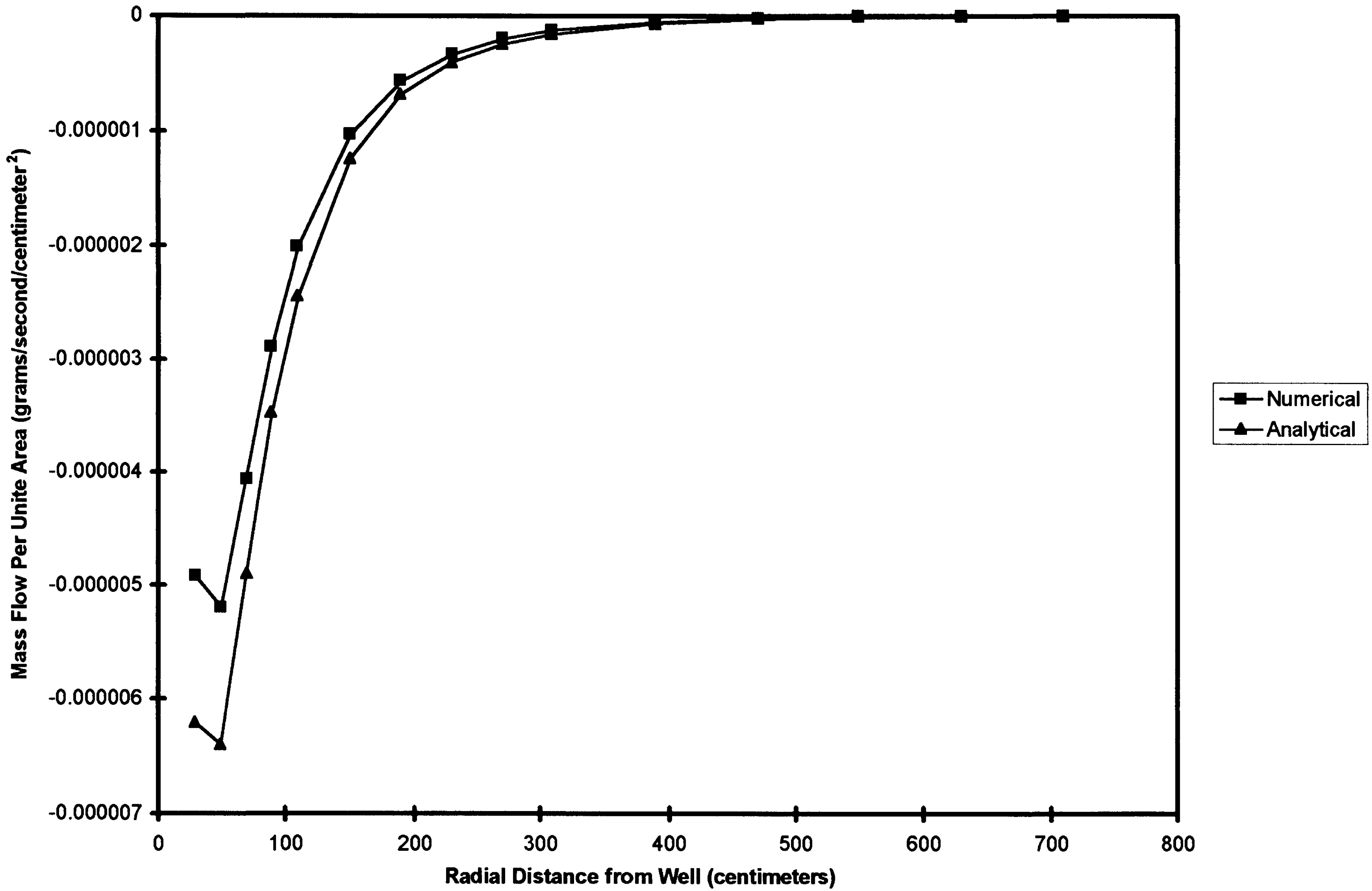

Figure 12.--Numerical and analytical horizontal flow predictions at 50 centimeters below grade for domain open to atmosphere.

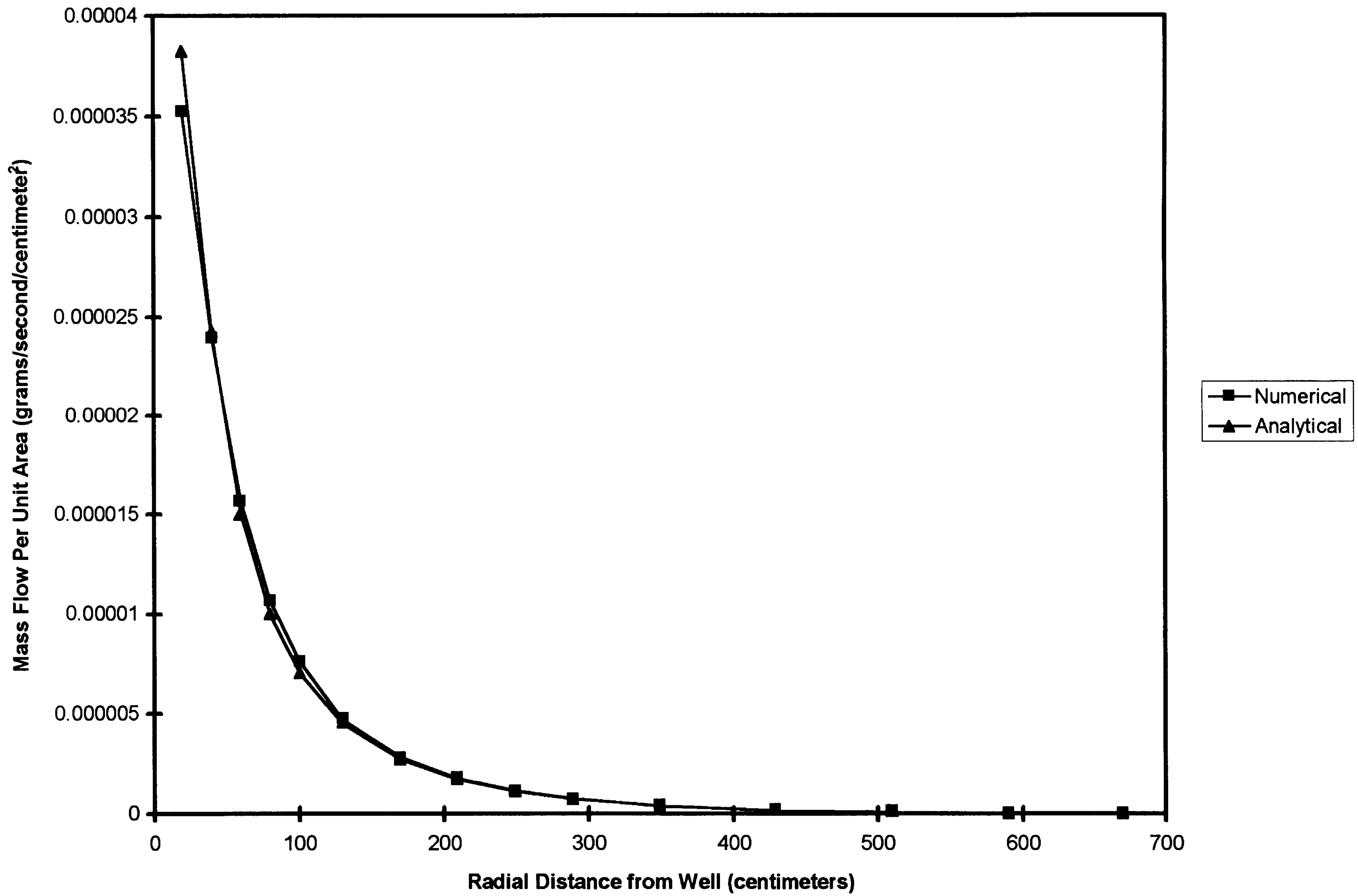

Figure 13.--Numerical and analytical vertical flow predictions at 50 centimeters below grade for domain open to atmosphere.

5.3.2 Input File

The data input file (DATAIRx.PRE) for the numerical air-flow analysis is as follows:

```
3 DIMENSIONAL AIR FLOW ANALYSIS (DOMAIN SEPARATED FROM ATMOSPHERE)
13 LAYERS, 41 ROWS, 41 COLUMNS
    1    1    1    1    1    1    1
        13        41        41         1
         1         1         0
         1
      1.00
    1   21   21   21   21    6    8     0.900
   3600.00         1       1.0
         1
    3020.0        1(6F10.1)
     160.0     160.0     160.0     160.0     160.0      80.0
      80.0      80.0      80.0      80.0      40.0      40.0
      40.0      40.0      40.0      20.0      20.0      20.0
      20.0      20.0      20.0      20.0      20.0      20.0
      20.0      20.0      40.0      40.0      40.0      40.0
      40.0      80.0      80.0      80.0      80.0      80.0
     160.0     160.0     160.0     160.0     160.0
    3020.0        1(6F10.1)
     160.0     160.0     160.0     160.0     160.0      80.0
      80.0      80.0      80.0      80.0      40.0      40.0
      40.0      40.0      40.0      20.0      20.0      20.0
      20.0      20.0      20.0      20.0      20.0      20.0
      20.0      20.0      40.0      40.0      40.0      40.0
      40.0      80.0      80.0      80.0      80.0      80.0
     160.0     160.0     160.0     160.0     160.0
       0.0      10.0      20.0 1.000E-10
         1     260.0
         1        13     260.0 1.000E-08  1.0 2.000E-08 0.30
```

5.3.3 Mass Balance for the Numerical Simulation

The following results of the numerical simulation summarize mass flow rates for air entering and exiting the model domain.

Mass Balance / Well / Unit Output for Domain Separated from Atmosphere

Mass flow into domain is positive
Mass flow out of domain is negative

Mass balance output for time step : 1	
Mass flow rate through model atmospheric layer	: 0.5811e+00 g/sec
Mass flow rate through left side of model domain	: 0.9815e-01 g/sec
Mass flow rate through back side of model domain	: 0.9815e-01 g/sec
Mass flow rate through right side of model domain	: 0.9815e-01 g/sec
Mass flow rate through front side of model domain	: 0.9815e-01 g/sec
Total mass flow rate across model boundaries	: 0.9737e+00 g/sec
Total mass flow rate through wells / trenches	: -0.9737e+00 g/sec
Flow across boundaries - flow through wells/trenches	: 0.3278e-06 g/sec
Percent air recharge from atmosphere	: 59.68 %
Percent air recharge from lateral boundaries	: 40.32 %
Normalized mass balance (flow in-flow out)/total flow	: 0.00 %
Mass flow rates through wells/trenches for time step : 1	
Mass flow rate through well number 1	: -0.9737e+00 g/sec
Volumetric flow rates through wells/trenches for time step : 1	
Volumetric flow rate through well number 1	: -0.8728e+03 cm^3/sec
Pressure in wells / trenches for time step : 1	
Pressure in well number 1	: 0.9000e+00 atm

5.3.4 Comparison of analytical and numerical solutions

The mass flow rate out of the well (0.974 g/s) was used as input to the analytical model. Model predictions from the analytical solution were compared with the numerical predictions for pneumatic pressure, horizontal air-flow rates, and vertical air-flow rates at 50 centimeters below grade. Flow output was normalized to specific discharge for the numerical solution by dividing by the area of a face. The pressure comparison between the analytical and numerical solutions is illustrated in figure 14. The horizontal component of mass flow comparison between the numerical and analytical solutions is illustrated in figure 15. The vertical component of mass flow comparison between the numerical and analytical solutions is illustrated in figure 16. The fit illustrated in figures 14 through 16 indicates that the numerical solution was implemented properly.

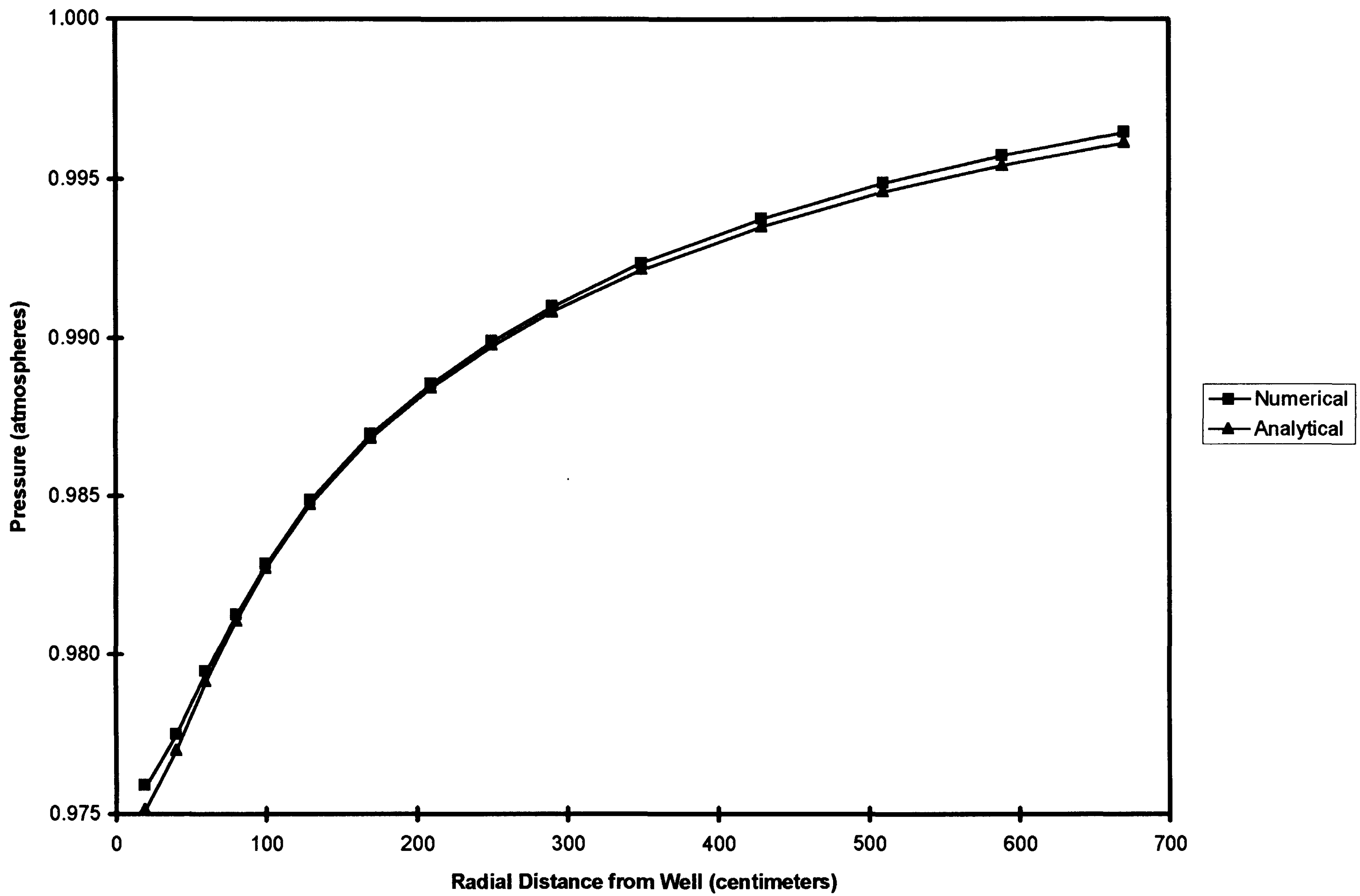

Figure 14.--Numerical and analytical pressure predictions at 50 centimeters below grade for domain separated from atmosphere.

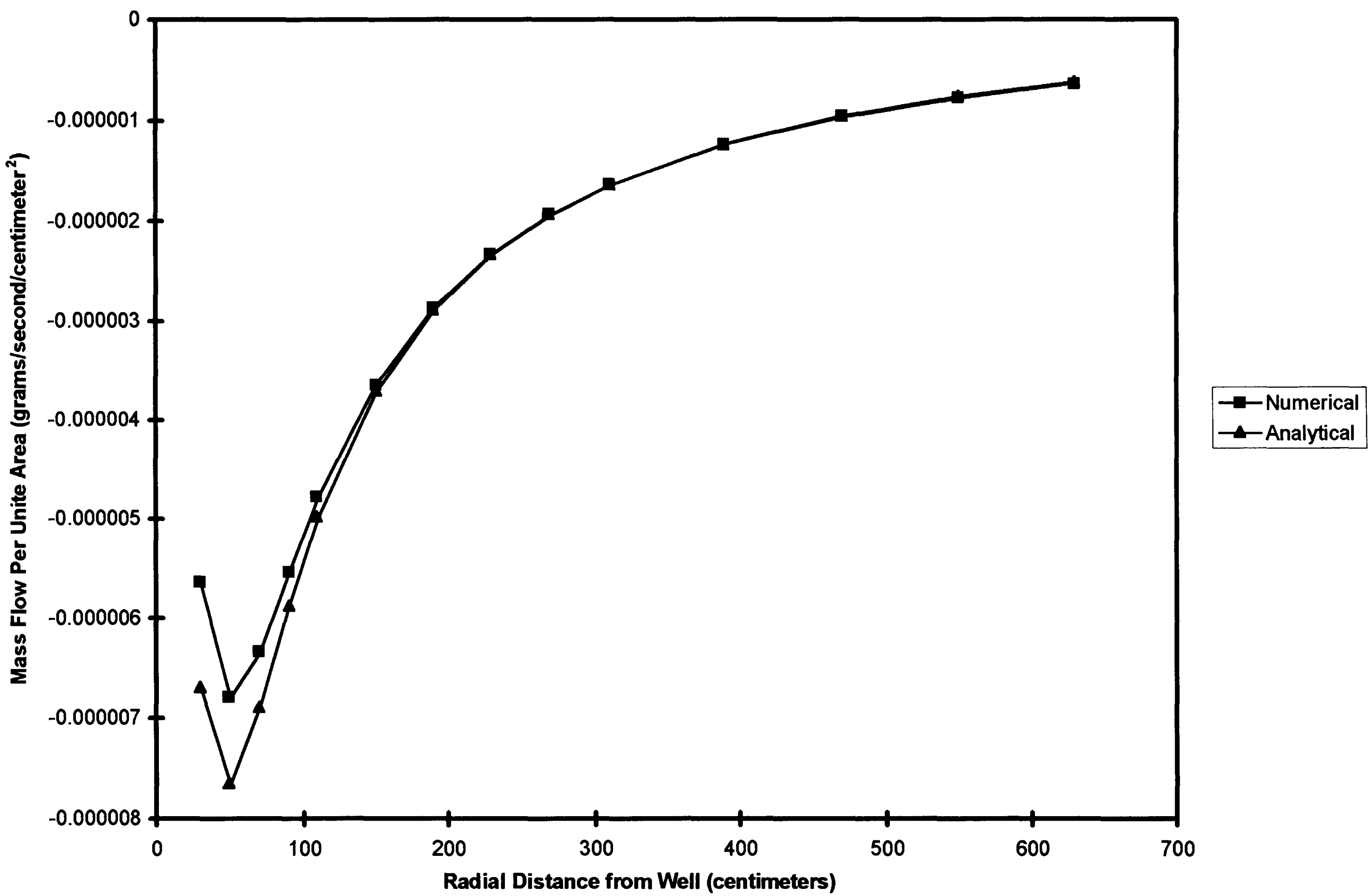

Figure 15.--Numerical and analytical horizontal flow predictions at 50 centimeters below grade for domain separated from atmosphere.

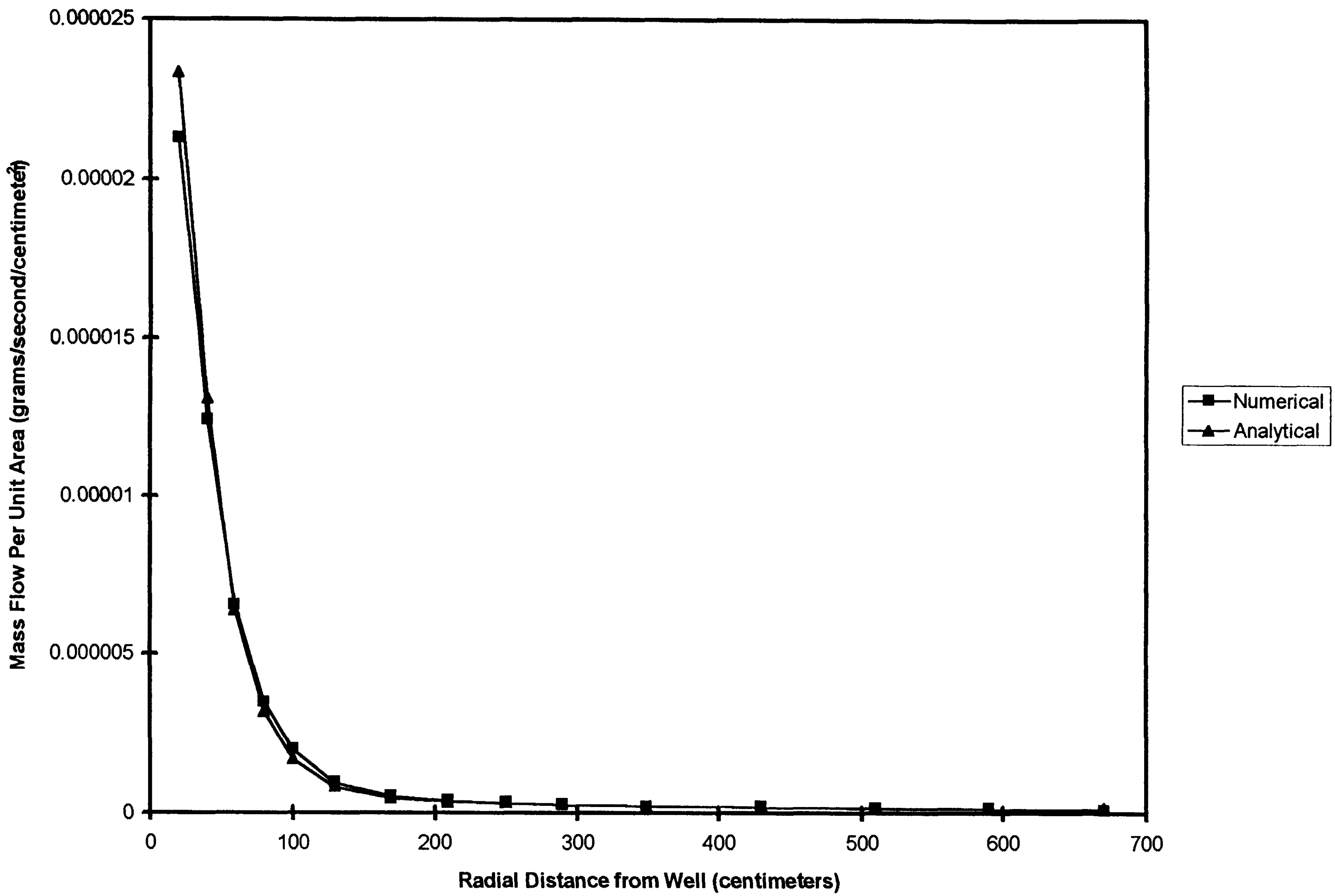

Figure 16. Numerical and analytical vertical flow predictions at 50 centimeters below grade for domain separated from atmosphere.

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