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BAROMETRIC PRESSURE TRANSIENT TESTING
APPLICATIONS AT THE NEVADA TEST SITE:
NUCLEAR CHIMNEY ANALYSIS

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FINAL REPORT

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CHAPTER I

INTRODUCTION AND BACKGROUND

The processes involved in creating nuclear chimneys in an alluvial or volcanic environment may create a wide distribution of rubble sizes ranging from coarse rubble, cobbles, and boulders, to fines. Most estimates of chimney permeability prior to the 1970's have been either very qualitative or based on a model of particle size distribution in samples taken from a chimney. The latter method has suggested that chimney permeability could approach one megadarcy, a value roughly five orders of magnitude greater than the typical surrounding undisturbed material (Rodean, 1965).

During the early 1970's, an effort was made by the Lawrence Livermore National Laboratory to reduce the uncertainty in both undisturbed alluvium and chimney permeability by carrying out pressure transient tests in-situ. These included air injection tests (Morris, et al., 1971; Rozsa, 1971; Snoeberger, et al., 1971) and passive in-situ chimney and undisturbed alluvium pressure response to atmospheric pressure variations at the surface (Snoeberger, et al., 1973; Snoeberger, et al., 1974; Rozsa, et al., 1974; Snoeberger, et al., 1974; Snoeberger, et al., 1972).

The basic concept is to interpret the measured surface and in-hole data in terms of a chimney model. Target parameters, namely permeability and hydraulic diffusivity, are the same as those in conventional air injection testing. Results of several of these tests are shown in Table 1.1. Three observations of some importance can be made from this table: (1) it is unlikely that chimney permeability will exceed one or two hundred darcies, (2) the differences between alluvium permeability and chimney permeability are not great. Table 1.1 suggests differences of roughly one order of magnitude or less, and (3) there may be significant differences in permeability from one chimney to another. These differences are likely to be a function of depth, formation strength, and shot yield.

More recent barometric pressure transient tests (Hanson, 1984) include analysis of data taken in the fractured volcanics of the NTS mesa areas as well as additional results for alluvium in the playa regions. Table 1.2 summarizes these results. These results are similar to Table 1.1 for alluvium permeability and diffusivity (U2fe) but suggest an order-of-magnitude larger hydraulic diffusivity for fractured volcanics. These tests were carried out in partially cased but otherwise open holes sealed from the atmosphere. As a result, the interpretation of the data was subject to more uncertainty, in terms of solution uniqueness, than the air injection and barometric tests reported in Table 1. However, two observations tend to give support to these data: (1) the computed diffusivity and permeability for the alluvium test

TABLE 1.1

Results of Historic Pressure Transient Testing at the Nevada Test Site

Site ¹	Area	Material/ region	Permeability $\mu\text{m}^2(\text{d})^2$ ²	Pressure diffusivity (m^2/s)	Test date	Remarks	Ref.
USPTS-cXY 30,5	3	Alluvium Vitric tuffs G. C. ashfall tuff Undifferentiated tuffs Carbonate rock	8.1 12.7 3.9 2.5 <2.0		July 7-14, 1971	Radial steady state, Air injection.	12
U10AM-5	10	Alluvium	8-16		July 20-21, 1971	Radial steady state, Air injection.	10, 11
CB-1, DH-3 and 4 DH-3, recalcd	10	Chimney in alluvium	23-38 62 ^d	1.0	May 19-25, 1972	Atmospheric- pressure method.	13 3
CB-2, DH-5 DH-5, recalcd	2	Chimney in alluvium	19 ^d 12 ^d	0.2	March and April, 1973	Atmospheric- pressure method.	1 3
CB-3, DH-6 DH-6 recalcd	2	Chimney in alluvium	33-66 56 ^d	0.5-1.0 1.0	Nov. 23- Dec. 22, 1973	Atmospheric- pressure method.	2 3
CB-4, DH-7 and DH-8	9 9	Alluvium and chimneyed tuff Surface alluvium	7 ^d 7 ^d	0.1 0.1	Feb. and March, 1974	Atmospheric- pressure method (no surface collapse).	4
CB-5 and DH-10	2 2	Alluvium Surface alluvium	41 ^d 70 ^d	0.6 1.0	July-Oct., 1974	Atmospheric- pressure method.	

¹CB numbers are sequential test-site numbers. DH numbers are sequential hole numbers, one or more per test location.

²Since 1 darcy = $0.987 \mu\text{m}^2$, the numbers in this column are essentially also in darcies.

³G. C. signifies Grouse Canyon.

^dPorosity of 0.3 used arbitrarily to obtain these values from the pressure diffusivity.

at U2fe is consistent with previous alluvium tests and (2) the calculated permeability in the volcanics is consistent with previous (Blankennegel and Weir, 1973) groundwater pump tests below the water table in the same area as the barometric tests. In any event, suggestions presented previously (Hanson, 1984) for resolving the question of model uniqueness for the open-hole barometric tests should be pursued vigorously.

It is clear from the data presented above that the possibility of radioactive gas leaks from the fractured volcanics in the NTS mesa areas may be significantly higher than in the playa regions simply due to the inferred large hydraulic diffusivities. Gas overpressure due to heating and compaction at the shot point will be driven away from the shot point. This gas will migrate through the overlying formation in a darcy-flow fashion which is governed by the hydraulic diffusivity. The higher the diffusivity, the more easily the formation can transport the gas. Furthermore, the high diffusivities suggest that surface barometric pressure fluctuations can penetrate to considerable depths - easily as deep as the shot point itself. The subsequent small, but pervasive, gas velocities will have the effect of increasing the dispersivity of the gas which may enhance the migration of the gas to the surface.

A correlation of surface barometric pressure fluctuation with surface radiation level has been recently observed in a mesa area of the NTS (Hearst, 1985). This mechanism of radioactive gas transport has not been studied in any detail historically. The fact that barometric pressure fluctuations are not a temporally limited driving force as is the shot point overpressure suggests that this mechanism may be quite important when considering the long term containment of radioactive gas following an underground nuclear test.

In the following, past investigations of barometric pressure testing of NTS nuclear chimneys will be reviewed. This review will include the models used in the interpretation, methods of analysis, and results. New and more sophisticated analytic and semi-analytic models will be presented and applied to both historical data and new data taken for this current project. An interpretation technique based on non-linear least squares methods will be used to analyze this data in terms of historic and more recent chimney models. Finally, a detailed discussion of radioactive gas transport due to surface barometric pressure fluctuations is presented. This mechanism of transport, which we refer to as "barometric pumping", is presented in terms of conditions likely to be encountered at the NTS. The report concludes with a discussion of the current understanding of gas flow properties in the alluvial and volcanic areas of the NTS, and suggestions for future efforts directed toward increasing this understanding are presented.

TABLE 1.2

Values of Diffusivity and Permeability at U2fe, U19ac,
and U20ai (from Hanson, 1984)*

Hole	Diffusivity (m**2/s)	Uncertainty (m**2/s)	Permeability (Darcy)	Comment
(A) Half-Space Models				
U2fe	1.3	0.03	30	[a]
U19ac	6.3 -	0.19 -	15 -	[b]
	25.5	1.15	60	
U20ai	4.2	0.07	10	[c]
(B) Multi-Layer Models				
U2fe	(0 - 334 m.)		36	[d]
	(334 m. -)		58	[d]
U19ac	(0-395 m.)		46	[e]
	(395 m. - 530 m.)		13	[f]
	(530 m. -)		22	[g]

[a] Homogeneous, isotropic half-space 1-D (vertical average) model. Assumed formation porosity 0.093 (alluvium)

[b] Homogeneous, isotropic half-space 1-D (vertical average) model. Assumed formation porosity 0.01 (volcanics). Large variation in diffusivity due to change in surface permeability from precipitation.

[c] Homogeneous, isotropic half-space 1-D (vertical average) model. Assumed formation connected porosity 0.01 (volcanics)

[d] Multi-layer model (finite difference) - both intervals are in alluvium

[e] Timber Mountain Tuff - assumed formation connected porosity 0.01 (volcanics)

[f] Paintbrush Tuff - assumed formation connected porosity 0.01 (volcanics)

[g] Rhyolite lava - assumed formation connected porosity 0.01 (volcanics)

* Open hole analysis - downhole high precision quartz pressure gauge suspended in a partially cased, but otherwise open hole

CHAPTER II

PART 1:

HISTORIC ANALYSES OF BAROMETRIC PRESSURE TRANSIENT TESTS IN NUCLEAR CHIMNEYS

Several investigations using barometric pressure transient testing for the purpose of evaluating nuclear chimney permeability have been made in the past (Snoeberger, et al., 1973; Rozsa, et al., 1974; Rozsa, et al., 1975), all of which were carried out in the playa areas of the NTS (Area 2, Area 9, and Area 10). In-hole pressure measurements were made through a partially cased slant hole intersecting the chimney-formation boundary at depth. A tube, grouted in the full length of the hole served as the conduit for the subsurface pressure signal to the surface pressure gauge. Surface and below-surface pressure were monitored by pressure transducers (1) in contact with the surface atmosphere and (2) connected at the surface with a tube going the length of the hole which is perforated at depth. Perforations were over a very limited depth interval to approximate a "point-response" sensing port. Figure 2.1 shows a typical chimney-slant hole-surface sensor geometry. All of the historic chimney data was acquired with a similar grouted in tubing.

This barometric pressure data was interpreted in terms of relatively simple chimney models (see Chapter III). The most common model used was a homogeneous and isotropic half-space. Gas flow was constrained to be one-dimensional in the vertical direction. This model presupposed that the chimney and surrounding formation had identical gas flow properties. The one other model used in interpretation was termed the "composite" model (Rozsa, et al., 1974), which again assumed one-dimensional flow (vertical) but broke the half-space into two distinct layers. The top layer, associated with the nuclear chimney, had one set of gas flow parameters and the bottom layer, associated with the surrounding formation, had another set of gas flow parameters. For the case in which the lower layer had zero permeability, the interface between the two layers represent a "no-flow" boundary. Thus, under this constraint, the composite model was referred to as a "composite no-flow" model. The derivation of this model is given elsewhere (Carslaw and Jaeger, 1959).

The theoretical formulation of all historic work and the present project, to be discussed later, is based on a linearized pressure diffusion equation, which assumes that the pressure perturbation due to surface barometric pressure variations is small compared with the static pressure due to the weight of the atmospheric column. This is an excellent approximation since typical values of the perturbation are less than 0.1 psi and the static pressure is on the order of 14 psi. Details of the linearization procedure are straight forward (see for example Sherwood, 1974) and are not presented here.

Figure 2.1. Typical slant-hole geometry used to access subsurface barometric pressure variation. Historical chimney data (DH3, DH5, DH6, DH7, and DH9) isolated the extent of the subsurface spatial port by grouting and perforating. Recent chimney data (U2fa, U2ff, U2ev, and U19ac) left hole from bottom of casing to bottom of slant hole open to formation.

The original historic pressure data was not available from these chianneys (Hearst, 1985). Also, the chianneys under consideration were designated with somewhat cryptic titles, making impossible to be able to locate these chianneys within the NTS more closely than area designation. We assume that these designations were for security purposes. In any event, the usefulness of a reinterpretation of this data is somewhat limited due to the fact that the location of these holes is presently not known. However, for the purpose of validating past interpretation results, and for extending the data base for chianney barometric pressure analysis, we digitized all of the above chianney data from the respective publications. Only those data which were judged suitable, in terms of published graphical resolution and available information regarding geometry of the slant hole and chianney, were digitized. A total of five chianneys, which have been analyzed historically, passed the above requirements. Their designations, as per the respective publications describing past analyses, are: DH3, DH5, DH6, DH7, and DH9.

The data was digitized using a Hewlett-Packard 7470A pen plotter/digitizer. Only inflection points were digitized, resulting in an unevenly spaced (in time) data set. Since subsequent analysis requires evenly spaced data, the data were linearly interpolated to an even spacing of 1/2 hour. All pressure data in the original publications were recorded and presented in voltage units rather than pressure units. This poses no problem as long as consistent units are maintained in the analysis. Therefore, we kept the pressure data in the original units of volts. The transducers were set to have a full-scale output of 0 to 10 volts over the pressure range 12.2 to 12.8 psia. The transducers had an absolute accuracy and precision of (+/-) 0.00833 psi and (+/-) 0.00167 psi, respectively (Snoeberger, et al., 1973).

Figures 2.2 through 2.6 show the digitized surface and downhole pressure data recorded at chianneys DH3 - DH9, respectively. Chianneys DH3, DH5, and DH6 were analyzed historically using both the infinite half-space model and the composite model (Rozsa, et al., 1974). These analyses consisted of carrying out a series of forward models on each chianney until the rms difference between the predicted in-chianney pressure record and measured in-chianney pressure record was minimized. In some cases, the rms fit was carried out "visually" and in other cases, the rms value was computed.

Results of these experiments are given in Table 2.1. The calculated permeabilities assume that the static gas pressure is 85 kPa and the gas viscosity is 0.00002 Pa.sec. With these values, the relationship between diffusivity and permeability is simply: $k(\text{Darcies}) = (\text{diffusivity} (\text{m}^2/\text{hr}) \times \text{porosity}) / 15.1$. We have taken porosity to be 0.2 in the following. The results are based on the infinite half-space model. The authors of these results report that "there was no significant difference between the no-flow composite model and the infinite half-space model".

FILES DH3SURB.DAT (SOLID), DH3DOWNB.DAT (DASHED)

HANSON & ASSOCIATES
CONSULTING GEOPHYSICISTS

Figure 2.2. Measured surface (solid) and downhole (dashed) pressure - DH3.

Figure 2.3. Measured surface (solid) and downhole (dashed) pressure - DH5.

Figure 2.4. Measured surface (solid) and downhole (dashed) pressure - DH6.

Figure 2.5. Measured surface (solid) and downhole (dashed) pressure - DH7.

Figure 2.6. Measured surface (solid) and downhole (dashed) pressure - DH9.

TABLE 2.1

Historically Computed Chimney Diffusivities

Chimney	Sensor Depth (m)	Diffusivity (m ² /hr)	Permeability (Darcies)
DH3	165	2882	38
DH5	216	533	7
DH6	340	3472	46
DH7	220	396	5
DH9	270	2315	31

The sensor depth referred to in the above table refers to the depth at which the subsurface pressure is monitored, and not the actual physical depth of the sensor. As mentioned previously, both pressure measurements are taken at the surface.

It is fairly obvious that the differences in diffusivity from location to location can be large, as high as a factor of almost 10. No correlation of diffusivity with depth is apparent in the results. One might expect such a correlation from the expected decrease in permeability with depth of compacted sediments. The lack of correlation can probably be attributed to two causes: (1) differences in site-specific rock strength and shot yield which may result in differing chimney gas flow properties and (2) variations in gas flow properties due to differences in local geologic setting. Indeed, chimney DH7 did not propagate to the surface whereas the other chimneys did. An interesting study, should the locations of these chimneys be determined, would be to see if the local rock properties and/or geologic setting could explain some of the above differences.

Some of the historic investigations also applied a much more sophisticated numerical model (TRUMP) for analyzing the data (Rozsa, et al., 1974). No specifics regarding whether or not this model accounted for stratigraphy of the adjacent formations or depth-dependent permeability within the chimney. Indeed, we do not know for sure that the model was set up to include both radial and vertical gas flow, although we suspect that it was. Only a few forward runs were made using TRUMP due to the large amount of computer time required. Values of diffusivity computed from the simple infinite half-space model were used in the forward models of TRUMP, and the computed in-chimney pressure record compared with the measured in-chimney record. The results of the numerical model were reported concisely: "no significant

differences were observed between TRUMP and the infinite half-space model".

Figures 2.7 - 2.11 show the amplitude spectra of the surface and downhole pressure signals for DH3 - DH9, respectively. These figures are presented here primarily to underscore the significant signal component at the tidal frequencies (see also, Hanson, 1984). However, as will be shown later, interpretation of chimney data can be carried out in the frequency domain as well as the time domain.

The specific mathematical models used to obtain the above results are discussed in the next chapter.

Figure 2.7a. Amplitude spectrum of surface barometric pressure record - DH3.

Figure 2.7b. Amplitude spectrum of downhole barometric pressure record - DH3.

Figure 2.8a. Amplitude spectrum of surface barometric pressure record - DHS.

Figure 2.8b. Amplitude spectrum of downhole barometric pressure record - DH5.

Figure 2.9a. Amplitude spectrum of surface barometric pressure record - DH6.

Figure 2.9b. Amplitude spectrum of downhole barometric pressure record - DH6.

Figure 2.10a. Amplitude spectrum of surface barometric pressure record - DH7.

Figure 2.10b. Amplitude spectrum of downhole barometric pressure record - DH7.

Figure 2.11a. Amplitude spectrum of surface barometric pressure record - DH9.

Figure 2.11b. Amplitude spectrum of downhole barometric pressure record - DH9.

PART 2:

RECENTLY ACQUIRED CHIMNEY DATA AT: U2fa, U2ff, U2ev, and U19ac

During the period 1984-1985, surface and subsurface barometric pressure fluctuations were monitored at nuclear chimneys U2fe, U2ff, U2ev, and U19ac. Pre-shot barometric data has been taken at two of the sites, U2fe and U19ac, making these sites of particular interest in comparing pre- and post-shot gas flow parameters. The subsurface data was acquired in a manner similar to the historical chimney data: namely, accessing the subsurface via a partially cased slant hole drilled to intersect the chimney at a depth near the bottom of the chimney. Unlike the historical data, however, the slant hole section below the casing was maintained open and was not grouted in to isolate the subsurface pressure measurement to a "point-response" port. Specifics of estimated chimney radius, casing length, slant hole depth, and depth to water table are given later (Table 4.2).

As will be discussed further in Chapter III, leaving the slant hole section beneath the casing open severely limits the sophistication of the interpretation model in that it not only breaks the cylindrical symmetry of the gas flow geometry in and about the chimney but also increases the problem of establishing a unique solution (see Hanson, 1984, for a discussion) in anything more complex than a homogeneous and isotropic half-space model.

High precision quartz pressure gauges (Paroscientific) were used to monitor pressure. These gauges were Paroscientific Digiquartz pressure gauges (Model 215) with a 0-15 psia full scale. Repeatability is 0.005% full scale and overall precision is better than 0.01%.

Figures 2.12 - 2.15 show the measured surface and downhole pressures at U2fa, U2ff, U2ev, and U19ac, respectively. Figures 2.16 - 2.19 show the amplitude spectra of the surface and downhole pressure variations from the mean for chimneys U2fa, U2ff, U2ev, and U19ac, respectively.

Table 2.2 shows the lithologic log at emplacement hole U2fa, which was completed entirely in the alluvium in Area 2. Figure 2.20 shows the surface effects map for U2fa. Figures 2.21 and 2.22 show geologic cross sections at U2fa. Table 2.3 shows the pre-shot lithologic log at emplacement hole U2ff. Figure 2.23 shows the pre-shot surface effects map at emplacement hole U2ff. Figures 2.24 and 2.25 show the geologic cross sections at U2ff.

Table 2.4 shows the pre-shot lithologic log at emplacement hole U2ev. Figure 2.26 shows the pre-shot surface effects map at U2ev. Figures 2.27 and 2.28 show the geologic cross sections at U2ev. Table 2.5 shows the lithologic log at emplacement hole

Figure 2.12. Measured surface (solid) and downhole (dashed) barometric pressure - U2fe.

Figure 2.13. Measured surface (solid) and downhole (dashed) barometric pressure - U2ff.

Figure 2.14. Measured surface (solid) and downhole (dashed) barometric pressure - U2ev.

Figure 2.15. Measured surface (solid) and downhole (dashed) barometric pressure - U19ac.

Figure 2.16a. Amplitude spectrum of surface barometric pressure record - U2fe.

Figure 2.16b. Amplitude spectrum of downhole barometric pressure record - U2fe.

Figure 2.17a. Amplitude spectrum of surface barometric pressure record - U2ff.

Figure 2.17b. Amplitude spectrum of downhole barometric pressure record - U2ff.

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Figure 2.18a. Amplitude spectrum of surface barometric pressure record - U2ev.

Figure 2.18b. Amplitude spectrum of downhole barometric pressure record - U2ev.

Figure 2.19a. Amplitude spectrum of surface barometric pressure record - U19ac.

Figure 2.19b. Amplitude spectrum of downhole barometric pressure record - U19ac.

U19ac. Figure 2.29 shows the location of U19ac within the Silent Canyon caldera, indicated by the heavy solid line. Figure 2.30 shows the geologic cross section at U19ac. The identification of geologic units in Figure 2.30 is given in Table 2.6.

Figure 2.20. Surface effects map for U2fe. (from Howard and Wagner, 1982)

Figure 2.21. Geologic cross section A-A' for U2fe. From Howard and Wagner, 1982).

Figure 2.22. Geologic cross section B-B' at U2fe. (from Howard and Wagner, 1982).

Figure 2.23. Surface effects map at U2if (from Clark and Howard, 1983)

Figure 2.24. Geologic cross section A-A' at U2ff (from Clark and Howard, 1983).

Location and Pre-event fracture map of the U2ev site

Figure 2.26. Surface effects map at U2ev (from Howard, 1983).

Figure 2.27. Geologic cross section A-A' at U2ev (from Howard, 1983).

Figure 2.28. Geologic cross section B-B' at U2ev (from Howard, 1983).

Figure 2.29. Pahute Mesa Drill Hole Location Map. (Arrow indicates location of U19ac - from Howard, 1984).

A NORTHWEST

A' SOUTHEAST

Figure 2.30. Geologic Cross Section A-A' Through U19ac. (From Howard, 1984).

TABLE 2.2

Lithologic Log - U2fe
(from Howard and Wagner, 1982)

DM 82-64
 Page 21

<u>DEPTH (m)</u>	<u>DESCRIPTION</u>
	Alluvium 0 - 449.6 T.O.
0 - 335.3	Mixed alluvium, brown to gray-brown variable proportions of Paleozoic clastic and carbonate detritus and Tertiary tuff fragments, Paleozoic clasts are more abundant than tuff clasts, calcaceous sand-silt matrix, caliche rinds on clasts are common, the alluvium consists of alternating beds of sand and gravel, with locally very coarse boulder beds, CO ₂ ranges from 0.2 - 13.7%, and averages 6.0%.
335.3 - 378.0	Mixed alluvium, brown to gray-brown, tuff detritus comprises >75% of the sediment, and Paleozoic clasts <25%, alternating beds of sand and gravel, with local coarse boulder beds, caliche is less common than unit above, CO ₂ ranges from 0.3 - 3.3%, and averages 2.6%.
378.0 - 449.6 T.O.	Mixed alluvium, brown to light brown, highly tuffaceous, tuff detritus comprises 80-90% and Paleozoic clasts, 10-20% of the sediment, basalt fragments occur at 393 m, the sediment ranges from mostly gravelly sand at the top of unit to coarse gravels at the base, caliche is minor, CO ₂ ranges from 0.1 - 2.9%, and averages 0.4%.
JLW 10/11/82	Lithology is based on drill cuttings, sidewall samples, grain density and CO ₂ analyses, and gamma log and downhole movie interpretation.

TABLE 2.3

Lithologic Log - U2ff
(from Clark and Howard, 1983)

CP 83-16
Page 22

<u>DEPTH (m)</u>	<u>DESCRIPTION</u>
	Alluvium 0 - 366 (T.O.)
0 - 355	Mixed alluvium, tan to dark gray fragments dominantly angular, composed of 65% - 90% sand and 10% - 35% gravel, 65% - 85% of gravel consists of fragments of Paleozoic argillite, quartzite, limestone and dolomite. Slightly calcareous with calcine rinds on some fragments. Increasing amounts of buff fragments and crystals at lower depths.
355 - 366	Basal buffaceous alluvium, white to gray fragments dominantly angular, mostly sand with minor amounts of gravel, 90% buff fragments, 10% fragments of Paleozoic argillite, quartzite, limestone and dolomite. Crystals abundant, biotite sparse, and magnetite common.
CSS: 12-16-81 Lithology is based on drill cuttings, sidewall samples, geophysical logs and CO ₂ analyses from sidewall samples.	

TABLE 2.4

Lithologic Log - U2wv
(from Howard, 1983)

CP 33-86
Page 21

<u>DEPTH (m)</u>	<u>DESCRIPTION</u>
0 - 310 m	Mixed alluvium, variable amounts of Paleozoic sedimentary clasts and Tertiary volcanic clasts. Clasts of Paleozoic rocks are mainly dark gray to light gray carbonate, with subordinate fine-grained to coarse-grained clastics. Basalt clasts occur locally near the base of the section. Detrital clasts range from well-rounded to angular, and calcine coatings are locally common. The sediments are mostly gravel from 0 - 140 m, gravelly sand from 140 - 274 m, and gravel from 274 - 310 m. Average $\sigma_g = 2.67 \text{ Mg/m}^3$ and average $\text{CO}_2 = 7.12\%$.
310 - 429 m	Mixed alluvium, but more tuffaceous than above. Clasts of Paleozoic rocks comprise $\sim 10\%$ of the sediment, and are mainly common throughout the section. Detrital quartz is common in the lower portion of the section. The sediments are mainly gravel and sandy gravel, becoming very coarse below 396 m. A coarse carbonate boulder bed occurs at 357 m. Average $\sigma_g = 2.60 \text{ Mg/m}^3$ and average $\text{CO}_2 = 1.98\%$.

JLW 5/11/83

This lithologic log was prepared using cuttings, gamma log, and downhole photography.

TABLE 2.5

Lithologic Log - U19ac
(from Howard, 1984)

<u>DEPTH (m)</u>	<u>LITHOLOGY</u>		
0 - 64.6	Tuff, ash-flow, devitrified, moderately welded.	} Anasazi Tanks Member	} Timber Mountain Tuff
64.6 - 71.0	Tuff, bedded, vitric, reworked and tuffaceous sandstone.		
71.0 - 402.0	Tuff, ash-flow, generally devitrified except for vitric top and base, partially to densely welded, contains upper vitrophyre (100.6 - 105.2m) and lower vitrophyre (375.7-383.4)	} Rainier Mesa Member	
402 - 431.3	Tuff, bedded, vitric to devitrified, slightly argillized, and calcareous in part, ash-fall and reworked.		- Bedded tuff
431.3 - 440.4	Lava flow, basalt, brecciated, vesicular, some caliche.		
440.4 - 531.9	Tuff, bedded, vitric to devitrified, zeolitized in part, ash-fall and reworked.		- Bedded tuff
531.9 - 701.2 TD	Lava flow, rhyolite, top 10 metres vitric frothy breccia; vitrophyric to about 556 metres; from 556 to 637 metres lava flow varies from devitrified to vitric, brecciated in part; from 637 to 701 metres flow is generally brecciated, devitrified, silicified and zeolitized in part.	}	- Pre-Pah Canyon rhyolite lava
LLNL RDMC (11-6-82) Revision of GN-23-80	Lithology from cuttings, geophysical logs and downhole photography (No faults observed).		

TABLE 2.6

Geologic Units for Figure 2.30

Quaternary units	
Qac	Alluvium and colluvium
Tertiary units	
Tma	Ammonia Tanks Member, Timber Mountain Tuff
Tmr	Rainier Mesa Member, Timber Mountain Tuff
Tp(Tb)	Bedded tuff associated the Paintbrush Tuff
Tpb	Tuff of Blacktop Buttes, tuffs and rhyolites of Area 20.
Tba	Basalt lava flow
Tpr	Pre-Pah Canyon rhyolite lava flow
Ta	Andesite lava flow
Trab	Bedded and ash-flow tuffs, tuffs and rhyolites of Area 20
Tral	Lower rhyolite lavas, tuffs and rhyolites of Area 20
Tdh	Lava and tuff of Dead Horse Flat.

CHAPTER III

ANALYTIC, SEMI-ANALYTIC, AND NUMERICAL CHIMNEY MODELS

Several barometric pressure chimney models have been used in the past to interpret measured pressure data in terms of gas flow parameters of the chimney and formation. Additional models have been developed during the course of this current project. The following presents the approximations and assumptions made and, in most cases, a brief derivation of each of the models. Some of the model derivations, most notably those in the frequency domain, are not presented for reasons of expediency. However, in these cases, the derivation is considered straight-forward and an appropriate derivation method is suggested. Computer programs for all of the models, both time- and frequency-domain, are given in Appendix I.

Historically, all of the chimney barometric pressure interpretation models have been derived in the time domain. Since the more sophisticated of these (for example, TRUMP) have been found to require excessive computer time, we have included equivalent models in the frequency domain. The primary motivation for this was to determine if calculations in the frequency domain might (1) speed up the interpretation and/or (2) supply a better insight into the interpretation. As will be shown, these goals are only partially achieved using this method.

All of the models presented start with the fundamental linearized diffusion equation given by:

$$\frac{\mu}{P_s} \frac{\partial P}{\partial t} = \vec{\nabla} \cdot \left(\frac{k}{\phi} \vec{\nabla} P \right)$$

where:

- μ = gas viscosity
- P_s = static (mean) gas pressure
- k = permeability
- ϕ = formation porosity
- P = formation gas pressure variation
- t = time

All of the chimney models presented in the following begin with this equation. Their differences are a result of applying different boundary conditions which reflect different chimney-

formation geometries.

It is emphasized that the dependent variable p in the above represents the pressure perturbation from the mean static pressure due to the surface barometric load variations, whereas the independent variable P_s represents the mean static load due to the weight of the atmosphere column. P_s can be taken to be the arithmetic mean of the barometric pressure record, or to good approximation, be taken to be 85 kPa. Additionally, all of the models presented assume that the gas (air) in the chimney-formation system is isothermal. As has been shown previously (Hanson, 1984), this assumption is acceptable except at some of the tidal frequencies associated with solar tides (eg. the K1, S1, S2, S3 frequencies).

3.1 Time Domain Models

3.1.1 Infinite Half-Space Model

We first consider the homogeneous and isotropic infinite half-space model. The model assumes that the gas flow properties of the chimney are identical to those of the surrounding formation. This is clearly an over-simplification. However, the model has been used extensively in historic work, and is also useful for obtaining a first estimate of gas diffusivity to be used as a starting value for more sophisticated models. Furthermore, as will be shown in Chapter IV, it is debatable whether the recently acquired barometric pressure data at several chimneys (U2fe, U2ff, U2ev, and U19ac) warrants a more sophisticated model. This is due primarily to the nature in which the data was acquired. Since the formation is homogeneous and isotropic, and the surface barometric load is considered to be spatially constant, the gas flow will be one-dimensional in the vertical direction. The appropriate diffusion equation under these restrictions reduces to:

$$\frac{1}{C} \frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial z^2} \quad (3-1)$$

where z is depth and where the new parameter, namely hydraulic diffusivity C , is defined by:

$$C = (k P_s) / (\mu \phi) \quad (3-2)$$

The boundary conditions for the infinite half-space model are given by:

$$p(z,t) = P_0(t), \quad z=0 \quad (3-3a)$$

$$p(z,t) \rightarrow 0, \quad z \rightarrow \infty \quad (3-3b)$$

where $P_0(t)$ is the surface pressure variation from the mean. The initial condition is given by:

$$p(z,t) = f(z), \quad t=0 \quad (3-4)$$

The initial vertical pressure distribution $f(z)$ is in fact unknown since, for any data set spanning a finite time period, the subsurface pressure at the beginning of the time period (ie. the initial pressure distribution for that particular data set) depends on the pressure history prior to that time. Interpretation methods must account for this lack of knowledge of the initial pressure distribution at the beginning of the data set time period. For time-domain models, the usual method is to "run" the model for an appropriate period of time, typically some fraction of the total data set time period, to a time $t=t^*$. Time t^* is then taken to be the initial time corresponding to $t=0$ in equation (3-4) and $p(z,t^*)$ is taken to be $f(z)$. The equilibration time t^* will of course depend upon the gas flow parameters of the model, which is what we are trying to determine in the first place. Therefore, it may be necessary to make several interpretation runs, each one using a value of t^* consistent with the computed gas flow parameters of the previous run. As will be shown later, the problem of unknown initial pressure distribution is more difficult to deal with for frequency-domain models.

The solution to equations (3-1) - (3-4) is easily found using the Laplace transform method. The diffusion equation is transformed into s -space, where s is the transform variable corresponding to time t :

$$\frac{\partial^2 \hat{p}}{\partial z^2} - \frac{s}{c} \hat{p} = -\frac{1}{c} f(z) \quad (3-5)$$

where the "hats" on p refer to Laplace transformed functions. Taking the initial formation pressure distribution $f(z)$ to be a constant f_0 for the moment, the general solution to equation (3-5) is easily determined to be:

$$\hat{p}(z, s) = A e^{-\sqrt{\frac{s}{c}} z} + B e^{\sqrt{\frac{s}{c}} z} + \frac{f_0}{s} \quad (3-6)$$

Using the boundary condition at infinite depth, we can immediately set B to zero to insure a finite solution at z infinite. The unknown coefficient A is determined by setting $z=0$ and introducing the surface boundary condition. The resulting solution, which is still in Laplace transform (s) space, is given by:

$$\hat{p}(z, s) = \hat{p}(0, s) e^{-\sqrt{\frac{s}{c}} z} + \frac{f_0}{s} \quad (3-7)$$

The above solution is easily transformed back into the time domain, for the case of a surface step function or surface delta function pressure history. These two particular surface loads are represented by their respective Laplace transforms:

(1) delta function: $\hat{p}(0, s) = 1$

(3-8)

(2) step function: $\hat{p}(0, s) = 1/s$

With these rather restrictive surface barometric pressure loads, the solution in Laplace transform space is easily transformed back to the time domain using a table of inverse Laplace transforms (for example, Abramowitz and Stegun, 1972):

(1) delta function:

$$p(z,t) - f_0 = \frac{z}{2\sqrt{\pi c t^3}} e^{-\frac{z^2}{4ct}} \quad (3-9)$$

(2) step function:

$$p(z,t) - f_0 = \operatorname{erfc} \left(\frac{z}{2\sqrt{ct}} \right)$$

The surface barometric pressure is in reality a function of time that bears little resemblance to either a step or delta function. However, for an arbitrary surface pressure perturbation history $p(0,t)$, the pressure history $p(z,t)$ can be obtained by convolving the delta function response at this depth with the surface pressure $p(0,t)$. The final solution for arbitrary surface pressure history is given by (see also Carslaw and Jaeger, p. 63):

$$p(z,t) = \frac{z}{2} \int_0^t \frac{e^{-\frac{z^2}{4c(t-\tau)}}}{\sqrt{\pi c(t-\tau)^3}} p(0,\tau) d\tau + f_0 \quad (3-10a)$$

Had the initial pressure distribution $f(z)$ not been a constant, the term f_0 in eq. (3-10a) would be changed to (see Carslaw and Jaeger, p. 357):

$$f_0 = \frac{1}{2\sqrt{\pi c t}} \int_0^\infty f(z') \left\{ e^{-\frac{(z-z')^2}{4ct}} - e^{-\frac{(z+z')^2}{4ct}} \right\} dz' \quad (3-10b)$$

Code module TDCMOD1, when linked with DRIVER1, will calculate both forward and inverse solutions to equation (3-10a). These modules are given in Appendix I. Note that for the purposes of numerical evaluation (ie. code module TDCMOD1), we have integrated eq. (3-10a) by parts to obtain a better behaved integrand in the convolution integral.

We have gone into some detail in the above derivation for the purpose of (1) introducing to those unfamiliar with the Laplace transform method the general technique and (2) for the purpose of outlining the general procedure for obtaining analytic and semi-analytic solutions for the chimney barometric pressure transient testing technique in the time-domain. All of the following time-domain solutions of this type are derived in an analogous manner.

3.1.2 Some Comments on Convolution

The general relationship between the surface barometric pressure perturbation and the subsurface response to this signal, for any flow model, is given by the expression:

$$p(\vec{r}, t) = \int_{-\infty}^t G(\vec{r}, t-\tau) p_0(\tau) d\tau \quad (3-11)$$

where:

Note that the subsurface pressure $p(x, y, z, t)$ depends on the entire history of the surface pressure to time t . The function $G(x, y, z, t)$ is called the time-domain transfer function or time-domain impulse response. It is simply the time history of the pressure perturbation at position (x, y, z) due to a surface pressure impulse (delta function). Equations (3-10a, b) explicitly give the impulse response for a homogeneous and isotropic half-space. Given an arbitrary input (ie. surface) signal $p(0, t) = p_0(t)$, the response is calculated through equation (3-10). The transfer function is independent of either the system input or system output.

Theoretical transfer functions (transfer functions calculated on the basis of an assumed model) in the time domain are easily calculated, as demonstrated in the simple half-space model presented above, and as will be demonstrated for other analytic and numerical chimney models presented later. It is also possible

to calculate actual transfer functions (transfer functions calculated on the basis of system input and output data) in the time domain given measured system inputs and outputs. This is a deconvolution process which can be carried out in several ways, none of which is trivial (Box and Jenkins, 1970) unless the initial subsurface pressure distribution can be taken to be either a constant in depth or identically equal to zero. However, if either of these assumptions can be made (an unlikely situation), the time-domain transfer function can be easily calculated using a simple recursive algorithm.

For practical situations, we never have an infinitely long surface pressure record. This situation can be accounted for by adding an additional unknown (error term) to the realizable convolution integral, as given by the following:

$$p(\vec{r}, t) = \int_0^t G(\vec{r}, t-\tau) p_0(\tau) d\tau + E \quad (3-12)$$

where:

$$E = \int_{-\infty}^0 G(\vec{r}, t-\tau) p_0(\tau) d\tau \quad (3-13)$$

Thus, in the time-domain, the error introduced by the finiteness of real data sets can be accounted for and minimized in a straight-forward manner. As discussed previously, the minimization of the error can be achieved by running the system model for a time $t=t^*$ so that $t=0$ (beginning of measured pressure record) approximates $(-\infty)$ in the above error term. Later on, we will consider analysis in the frequency domain. It is less obvious in the frequency domain how these kinds of uncertainties can be accounted for, as will be discussed later.

3.1.3 Infinite Half-Space Model with "No-Flow" Boundary

This particular model assumes again that the chimney and surrounding formation have identical gas flow properties as in the infinite half-space model presented above. However, at some depth L , there is a no-flow boundary. This boundary might represent the water table or a very tight formation underlying a more permeable formation. The no-flow boundary at $z=L$ is given

by:

$$\left. \frac{\partial p}{\partial z} \right|_{z=L} = 0 \quad (3-14)$$

The solution to equations (3-1), (3-3a), (3-4), (3-8), and (3-14), in Laplace transform space, where we have again assumed that the initial formation pressure distribution $f(z)$ is a constant, f_0 , is given by:

(1) delta function:

$$\hat{p}(z,s) - \frac{f_0}{s} = \frac{\cosh\left(\sqrt{\frac{s}{c}}[z-L]\right)}{\cosh\left(\sqrt{\frac{s}{c}}L\right)} \quad (3-15)$$

(2) step function:

$$\hat{p}(z,s) - \frac{f_0}{s} = \frac{1}{s} \frac{\cosh\left(\sqrt{\frac{s}{c}}[z-L]\right)}{\cosh\left(\sqrt{\frac{s}{c}}L\right)}$$

The inverse Laplace transform of the above is tedious to obtain in an analytic fashion and results in an infinite series which may prove tedious to compute. We therefore use a numerical inverse Laplace transform algorithm to cast the solution in the time domain. Several such algorithms exist. We have found that the Stehfest algorithm (Stehfest, 1970) is both fast and accurate.

Code module TDCMOD2, when linked with DRIVER1, will calculate the time-domain impulse response solution given by equation (3-15) and convolve the impulse response with an arbitrary surface pressure history. These modules are given in Appendix I.

3.1.4 Layered Half-Space Chimney Model

This model assumes that the chimney and surrounding formation have identical gas flow properties on a depth by depth basis. This model may be a rather inappropriate situation for an actual chimney-formation system, but it might be argued that the two

models presented previously are equally inappropriate. We also point out that this model is the most sophisticated model that can be justified for the analysis of recently acquired chimney data. This is discussed further in Chapter IV. We have therefore included this model for completeness. The solution of this model has been presented elsewhere (Hanson, 1984),

The method of solution to the 1-D flow layered half-space problem is similar to the solution given for the homogeneous half-space, with the exception that now, we have two additional boundary condition constraints. These constraints derive from the requirement of pressure continuity and mass flux continuity across the layer interfaces. Figure 3.1 shows the layered half-space geometry for n layers. The bottom of the n th layer is assumed to go to infinity. The mathematical statement of the problem is given as follows:

- (1) diffusion equation for each layer:

$$\frac{1}{C_i} \frac{\partial p_i}{\partial t} = \frac{\partial^2 p_i}{\partial z^2}, \quad z_{i-1} < z < z_i$$

$$i = 1, 2, \dots, n$$
(3-16)

- (2) initial condition for all layers and boundary condition at surface

$$p_i(z, t) \Big|_{t=0} = f_0, \quad i = 1, 2, \dots, n$$

$$p_i(z, t) \Big|_{z=0} = p_0(t)$$
(3-17)

- (3) lower boundary of bottom layer goes to infinity

$$p_n(z, t) \Big|_{z \rightarrow \infty} = 0$$
(3-18)

Figure 3.1. Geometry of layered half-space chimney model. Permeability and porosity are defined for each layer.

(4) pressure continuity across layer interfaces

$$p_i(z_i, t) = p_{i+1}(z_i, t), \quad i=1, 2, \dots, n \quad (3-19)$$

(5) mass flux continuity across layer interfaces

$$k_i \left. \frac{\partial p_i}{\partial z} \right|_{z=z_i} = k_{i+1} \left. \frac{\partial p_{i+1}}{\partial z} \right|_{z=z_i} \quad (3-20)$$

$i=1, 2, \dots, n$

Eqs. (3-19) and (3-20) represent the pressure and mass flux continuity constraints at the layer interfaces. Casting eqs. (3-16) through (3-20) in Laplace transform space, one can obtain a set of $2n-2$ equations representing the $2n-2$ unknowns. The latter are the set of layer coefficients $[A(1), B(1)]$, $[A(2), B(2)]$, $[A(3), B(3)]$, ..., $[A(n), B(n)]$, where each set of brackets $[\]$ represent a single layer in the n -layer half-space. The blanks in the brackets representing the surface layer (layer 1) and the bottom layer (layer n) are due to imposed boundary conditions on these layers, as will be seen in the following. The general solution for the i th layer (in Laplace transform space) is given by:

$$\hat{p}_i(z, s) = A_i e^{-\sqrt{\frac{s}{C_i}} z} + B_i e^{\sqrt{\frac{s}{C_i}} z} + \frac{f_0}{s} \quad (3-21)$$

$z_{i-1} < z < z_i$
 $i=1, 2, \dots, n$

Note that $B(n)$ is zero due to the requirement that the solution go to zero as depth goes to infinity. Also, $A(1)$ can be evaluated by noting that:

$$A_1 = \hat{P}_0(1) - B_1 = f_0/2 \quad (3-22)$$

where:

$$\hat{P}_0(1) = \begin{cases} 1, \text{ delta function} \\ 1/s, \text{ step function} \end{cases}$$

Combining eqs. (3-19), (3-20), and (3-21), we can set up an 2×2 matrix that "propagates" the layer coefficients downward. That is, given the coefficients for the i th layer, the coefficients for the $(i+1)$ th layer can be quickly evaluated with a simple matrix multiplication. With some algebra, it can be shown that:

$$\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} = M \begin{pmatrix} A_i \\ B_i \end{pmatrix} \quad (3-23)$$

where the "propagator matrix", M , is given by:

$$M = X^{-1}Y \quad (3-24)$$

in which:

$$X = \begin{pmatrix} x_{11}^i & x_{12}^i \\ x_{21}^i & x_{22}^i \end{pmatrix} \quad (3-25)$$

$$Y = \begin{pmatrix} y_{11}^i & y_{12}^i \\ y_{21}^i & y_{22}^i \end{pmatrix}$$

and where the matrix elements are defined by:

$$x_{11}^i = -k_{i+1} \sqrt{\frac{z}{c_{i+1}}} e^{-\sqrt{\frac{z}{c_{i+1}}} z_i}, \quad x_{21}^i = e^{-\sqrt{\frac{z}{c_{i+1}}} z_i}$$

$$x_{12}^i = k_{i+1} \sqrt{\frac{z}{c_{i+1}}} e^{\sqrt{\frac{z}{c_{i+1}}} z_i}, \quad x_{22}^i = e^{\sqrt{\frac{z}{c_{i+1}}} z_i}$$

$$y_{11}^i = -k_i \sqrt{\frac{z}{c_i}} e^{-\sqrt{\frac{z}{c_i}} z_i}, \quad y_{21}^i = e^{-\sqrt{\frac{z}{c_i}} z_i}$$

$$y_{12}^i = k_i \sqrt{\frac{z}{c_i}} e^{\sqrt{\frac{z}{c_i}} z_i}, \quad y_{22}^i = e^{\sqrt{\frac{z}{c_i}} z_i}$$

From a computational standpoint, it is most efficient to solve for all of the layer coefficients simultaneously. This is best achieved by noting from eqs. (3-23) - (3-25) that we can write, with some rearrangement:

$$\begin{pmatrix} (y_{12}' - y_{11}') & -x_{11}' & -x_{12}' & 0 & 0 & \cdots & 0 & 0 \\ (y_{22}' - y_{21}') & -x_{21}' & -x_{22}' & 0 & 0 & \cdots & 0 & 0 \\ 0 & y_{11}^2 & y_{12}^2 & -y_{11}^2 & -y_{12}^2 & 0 & 0 & \cdots & 0 \\ 0 & y_{21}^2 & y_{22}^2 & -y_{21}^2 & -y_{22}^2 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & y_{11}^n & y_{12}^n & -x_{11}^n & 0 \\ 0 & 0 & 0 & 0 & 0 & y_{21}^n & y_{22}^n & -x_{21}^n & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ A_2 \\ B_2 \\ A_3 \\ \vdots \\ B_n \\ A_{n+1} \end{pmatrix} \quad (3-26)$$

$$= -\hat{p}_0(z) (y_{11}', y_{21}', 0, 0, \dots, 0)^T$$

Eq. (3-26) is simply a set of simultaneous equations that can be solved by any number of methods for the unknown coefficients $(h(1), B(1)), 1=1, 2, \dots, n$. The $(n+1)$ th layer is a uniform layer of infinite thickness. Note that this system of equations is in Laplace transform space. It would be a tedious, if not impossible, task to analytically invert the solution. We therefore have employed a numerical Laplace transform technique (Stehfest, 1969; Crump, 1976) to obtain a usable solution in the time domain.

It should also be pointed out here that the solution derived on the basis of eq. (3-26) is appropriate only for the condition that the Laplace transform of the surface pressure, $P(t)$, is available. In the case of barometric pressure loading at the surface, this will not be the case. One way around this is simply to calculate numerically the Laplace transform of the surface pressure signal. In principle, this is straight forward. However, in practice, the sampling interval in time may preclude obtaining a reasonable precision in calculating the numerical Laplace transform. A better method is to calculate the impulse response of the layered half-space by assuming the surface pressure is a delta function in time. The Laplace transform of a delta function is simply the quantity 1, as noted previously. Once the impulse response is calculated, the pressure response at depth due to an arbitrary surface pressure history is determined by convolving the surface pressure with the impulse response. This method has been discussed previously for the infinite half-space model.

Code module TDCMOD6, when linked with DRIVER1, will calculate both the forward and inverse solutions to equation (3-26). These modules are given in Appendix I.

3.1.5 Cylindrical Chimney Model

The next chimney model to be considered is that of a vertical finite length chimney of constant radius and given gas flow properties embedded in a formation of different gas flow properties. A no-flow boundary is placed at $z=L$ in both the chimney and the formation. The principle purpose for the no-flow boundary is to make available the use of orthogonal functions in the solution. However, if the shot point is just above a water table, the model may be a reasonable approximation to the actual situation. Figure 3.2 shows the geometry of this model. The solution is similar to a solution obtained for heat flow in cylindrical coordinates (Peavy, 1968). In the following, we will refer to the formation as region I and the chimney as region II.

Figure 3.2. Geometry of cylindrical chimney model. Permeability and porosity are defined for both chimney and formation.

The linearized diffusion equation in cylindrical coordinates is given for both regions I and II by:

Region I:

$$\frac{1}{c_I} \frac{\partial p_I}{\partial t} = \frac{\partial^2 p_I}{\partial r^2} + \frac{1}{r} \frac{\partial p_I}{\partial r} + \frac{\partial^2 p_I}{\partial z^2} \quad (3-27)$$

Region II:

$$\frac{1}{c_{II}} \frac{\partial p_{II}}{\partial t} = \frac{\partial^2 p_{II}}{\partial r^2} + \frac{1}{r} \frac{\partial p_{II}}{\partial r} + \frac{\partial^2 p_{II}}{\partial z^2}$$

where r is the radial coordinate from the axis of the chimney. The boundary conditions at the interface between chimney and formation are given by:

(1) mass flux continuity:

$$k_I \left. \frac{\partial p_I}{\partial r} \right|_{r=r_w} = k_{II} \left. \frac{\partial p_{II}}{\partial r} \right|_{r=r_w} \quad (3-28)$$

(2) pressure continuity:

$$p_I|_{r=r_w} = p_{II}|_{r=r_w}$$

The boundary conditions at the surface and at the no-flow boundary are given by:

(1) surface pressure boundary condition

$$p_I(r, z, t) \Big|_{z=0} = p_{II}(r, z, t) \Big|_{z=0} = p_o(t) \quad (3-29)$$

(2) "no-flow" boundary condition:

$$\left. \frac{\partial p_I}{\partial z} \right|_{z=L} = \left. \frac{\partial p_{II}}{\partial z} \right|_{z=L} = 0$$

where $P_0(t)$ is the surface barometric pressure variation from the mean. Finally, the initial pressure perturbation at $t=0$ is taken to be zero.

The solution is cast as a series solution of orthogonal functions in the z -coordinate. In Laplace transform space, these solutions can be found to be:

$$\begin{aligned} \text{Region I. } \hat{p}_I(r, z, 1) &= \sum_{n=0}^{\infty} B_n K_0 \left(\sqrt{b_n^2 + \frac{1}{c_I}} r \right) \sin(b_n z) \\ &+ \hat{p}_{Ih}(z, 1) \end{aligned} \quad (3-30)$$

$$\begin{aligned} \text{Region II. } \hat{p}_{II}(r, z, 1) &= \sum_{n=0}^{\infty} C_n I_0 \left(\sqrt{b_n^2 + \frac{1}{c_{II}}} r \right) \sin(b_n z) \\ &+ \hat{p}_{IIh}(z, 1) \end{aligned}$$

where:

$$b_n = (n + 1/2) \pi / L$$

and where $\hat{p}_{Ih}(z, 1)$, $\hat{p}_{IIh}(z, 1)$ are the 1-D (vertical) solutions if chimney has the same properties as the formation, or if the formation has the same properties as the chimney, respectively. Thus, the part of the solution represented by the summations has to do with the pressure perturbation field caused by the existence of the chimney (for region I) and the existence of the formation (for region II). The coefficients (B_n, C_n , $n=0, 1, \dots$) are determined from the two boundary conditions at the chimney-formation interface given by equation (3-28). With some algebra, and using the orthogonality properties of the trigonometric functions, these coefficients can be found to be:

$$B_n = \frac{k_{II} \gamma_n I_1(\gamma_n r_w) \Delta_n(1)}{k_{II} \gamma_n K_0(\beta_n r_w) I_1(\gamma_n r_w) + k_I \beta_n K_1(\beta_n r_w) I_0(\gamma_n r_w)}$$

$$C_n = \frac{-k_I \beta_n K_1(\beta_n r_w) \Delta_n(1)}{k_{II} \gamma_n K_0(\beta_n r_w) I_1(\gamma_n r_w) + k_I \beta_n K_1(\beta_n r_w) I_0(\gamma_n r_w)} \quad (3-31)$$

where: $\gamma_n = \sqrt{b_n^2 + \frac{1}{c_{II}}} \quad , \quad \beta_n = \sqrt{b_n^2 + \frac{1}{c_I}}$

and where:

$$\Delta_n(1) = \frac{2}{L} \int_0^L [\hat{p}(z, 1) - \hat{p}_I(z, 1)] \sin(b_n z) dz$$

Again imposing the restriction that the surface pressure history is either a delta function or a step function, the integral $\Delta_n(1)$ is given by:

$$\Delta_n(1) = \hat{p}_0(1) \frac{2b_n}{L} \left\{ \frac{\left(\frac{1}{c_I} - \frac{1}{c_{II}} \right)}{\left(\left(\frac{1}{c_{II}} + b_n^2 \right) \left(\frac{1}{c_I} + b_n^2 \right) \right)} \right\} \quad (3-32)$$

where, for:

(1) delta function surface pressure: $\hat{p}_0(z) = 1$

(2) step function surface pressure: $\hat{p}_0(z) = 1/2$

The final solution for the formation pressure perturbation, evaluated at the formation-chimney boundary $r=r_w$, is given by:

$$\hat{p}_I(r, z, 1) = \hat{p}_0(z) \left\{ \frac{\cosh(\sqrt{\frac{z}{c_I}}(z-L))}{\cosh(\sqrt{\frac{z}{c_I}}L)} + \right.$$

$$\left. \frac{z}{L} \left(\frac{1}{c_I} - \frac{1}{c_{II}} \right) \sum_{n=0}^{\infty} \frac{b_n \sin(b_n z)}{(\beta_n \delta_n)^2 \left(1 + \frac{k_I \beta_n}{k_{II} \delta_n} \frac{K_1(\beta_n r_w) I_0(\delta_n r_w)}{I_1(\delta_n r_w) K_0(\beta_n r_w)} \right)} \right\}$$

(3-33)

The above solution is transformed back to the time domain using the Stehfest numerical Laplace transform inversion algorithm. Program module TDCMOD5, when linked with module DRIVER1, can calculate either the forward or inverse solutions to equation (3-33). Both of these modules are given in Appendix I.

Equation (3-33) suggests that, if the approximate chimney radius and depth to no-flow boundary are known, the system response is governed by three parameters: chimney diffusivity, formation diffusivity, and the ratio of (chimney permeability/formation permeability). If all three parameters are evaluated as a solution to the inverse problem, the permeability ratio will, when combined with the diffusivities, yield the ratio of (chimney connected porosity/formation connected porosity), although the porosities cannot be determined individually.

3.1.6 Finite Difference Model - Time Domain

The above analytic and semi-analytic models are useful for establishing initial estimates of gas flow parameters. However, at least for the forward problem of predicting subsurface pressure given formation and chimney gas flow parameters, these models are somewhat restrictive in terms of allowable complexity. We have therefore constructed a numerical model of gas flow in and about a chimney which can account for: (1) arbitrary location of bottom of chimney and depth of water table (ie. no-flow boundary), (2) vertical distribution of porosity and permeability within the chimney and (3) vertical distribution of porosity and permeability in the formation.

The numerical approach is based on a model presented by Prickett and Lonnquist (1971), with appropriate modifications to their model to represent the geometry of a chimney-formation system with spatially constant surface pressure load history. Innumerable descriptions of the finite difference method have been presented in the literature. We will not present another description here. However, Appendix II presents a detailed description of Prickett and Lonnquist's method which uses the iterated alternating direction implicit (IADI) numerical technique. This Appendix is included for those who may wish to better understand this particular method or who may wish to alter the code to address other problems.

The numerical approach solves the linearized diffusion equation in two dimensions (radial and vertical) subject to pressure and mass flux continuity boundary conditions at material interfaces. No-flow boundaries are set at prescribed a prescribed radial distance (large enough to simulate infinity) and at a

prescribed depth (corresponding to the location of the water table). The initial static pressure within the chimney-formation system is set to 85 kPa (in the forward model) or to either 85kPa or the seen of the measured pressure record (in the inverse model).

Figure 3.3 shows a generalized geometry of the chimney-formation geometry that can be addressed by the finite difference computer code contained in this report. The code can allow up to 10 distinct layers of different thicknesses within the chimney and formation. Within each of these layers, the chimney gas flow properties (porosity and permeability) can be different from the formation gas flow properties. The model assumes equi-spaced radial nodes within the chimney and geometrically increasing radial node spacing within the formation away from the chimney. Vertical node spacing is assumed to be uniform within each layer, but the vertical spacing can be different from layer to layer. Total number of radial nodes is limited to 20 and the total number of vertical nodes to 200. Precision is governed by a user-prescribed convergence criterion. Code module CHAN, when linked with RCHAN, calculates the forward solution using the alternating direction finite difference method. Code modules TDCA#1, when linked with TDCA#2, calculate both the forward and inverse solutions using the alternating direction finite difference method. A warning is in order here: using the finite difference model for the inverse problem can lead to a large expenditure of computer time.

The location of the subsurface pressure sensor (or sensing port) is determined by specifying a particular node by radial and vertical node index. This is a somewhat crude method of locating the downhole sensor. A better technique, easily implemented, is to specify the exact location of the downhole sensor and calculate the node locations accordingly. In this manner, a node location can be made to correspond exactly with the subsurface sensor location. As currently configured, each of the layers is assumed to be homogeneous and isotropic within the chimney or within the formation. The code is easily changed to lift this restriction (see Prickett and Lonnquist). Also, as currently configured, layer interfaces within the chimney must conform to layer interfaces within the formation, whether or not there are gas flow parameter differences across these interfaces. This can be relaxed in an easy fashion with appropriate "book-keeping" (see for example Program KOBRA (Modules 1 & 2), Hanson, 1934).

Figure 3.3. Geometry of chimney-formation system used in numerical (finite difference) model. For a given layer, permeability and porosity may be defined separately for chimney and formation.

3.1.7 Numerical Examples - Time Domain

An example of the time domain cylindrical chimney model was calculated for the purpose of validating both the finite difference chimney model (CHAN+RCHAN, TDCA#1+TDCA#2) and the analytic solution of the cylindrical chimney model (DRIVER1+TDCMODS). Figure 3.4 shows the geometry of this example. A 1 kPa surface pressure load was applied at $t=0$ and maintained for $t>0$. The sensor was located at the formation-chimney boundary at a depth of 100 m. The distance to the no-flow boundary was taken to be 300 m. and the chimney radius was taken to be 50 m.

Two cases were considered. In the first case, the formation permeability and porosity were taken to be 10 Darcy and 0.2, respectively, and the chimney permeability and porosity were taken to be 50 Darcy and 0.2, respectively. For the second case, the formation permeability was taken to be 50 Darcy and the chimney permeability was taken to be 10 Darcy. The chimney and formation porosity were both taken to be 0.2. For the numerical finite difference solution, 50 vertical nodes were used between the surface and depth $z=100$ m. Another 50 vertical nodes were used between depths $z=100$ m. and $z=300$ m. Ten radial nodes were taken in the chimney and the outer boundary (for the numerical solution) was 1 km. The time step used was 0.5 hour. The semi-analytic solution summation given by eq. (3-31) was truncated when the next term in the sum contributed less than 0.0001 of the sum to that point. The convergence criteria used for the alternating direction finite difference model was 1 Pa - that is, if at any step within the iteration, the maximum change in pressure for any of the nodes was less than 1 Pa, the solution was reached (by definition).

Figure 3.5 shows the sensor pressure history for the first 100 hours after the application of the surface pressure perturbation. Five terms were retained in the numerical Laplace transform inversion summation in the semi-analytic solution. Figure 3.6 shows the same result except that six terms were retained in the summation. Figure 3.6 shows the onset of the numerical stability associated with the numerical Laplace transform inversion. The Stehfest algorithm is such that the number of terms retained in the Laplace inversion should be roughly the number of significant digits the computer can retain. Had the code been run on a mainframe machine (as opposed to a micro), the number of terms could have been increased before the onset of this instability. In any event, the results indicate that both the numerical and semi-analytic solutions are computing the same result. Figure 3.7 shows the pressure history at the sensor for case II.

We attribute the differences between the numerical and semi-analytic solutions discussed above principally to the semi-analytic solution. We recommend that the algorithm used for the evaluation of the Bessel functions under the summation be improved, and that, unless a machine is available that supports at least 12 significant digits, all calculations be carried out in double precision.

Figure 3.4. Chimney-formation-sensor geometry used for comparison of semi-analytic and numerical time-domain cylindrical chimney models.

Figure 3.5. Comparison of numerical (dashed) and semi-analytic (solid) cylindrical chimney models - Case I, time domain. (Number of terms retained in Laplace inverse = 5).

Figure 3.6. Comparison of numerical (dashed) and semi-analytic (solid) cylindrical chimney models - Case I, time domain. (Number of terms retained in Laplace inverse = 6).

Figure 3.7. Comparison of numerical (dashed) and semi-analytic (solid) cylindrical chimney models - Case II, time domain.

3.2 Frequency Domain Models

3.2.1 General Discussion

Past experience with the use of finite difference models to calculate barometric pressure response in the subsurface has indicated that this approach is computationally slow in the time domain (Hanson, 1984; Rozsa, et al., 1974). One possible alternative approach which might speed up computation time is by carrying out the analysis in the frequency domain. The logic behind this hypothesis is that a convolution in the time domain is equivalent to a product in the frequency domain. Since a single product requires much less computation than a sum of products, the computational advantages are clear.

Another motivation for carrying out the analysis in the frequency domain is the fact that different frequencies of the surface pressure signal have different penetration depths, depending on the gas flow properties of the formation. Lower frequencies penetrate deeper than higher frequencies. It may be reasonable to assume that this kind of information will allow more information about the depth dependence of the gas flow properties to be determined.

Finally, it must be pointed out that the inverse problem of inferring gas flow properties (ie. permeability, diffusivity) is highly dependent upon the spectral content of the input and output signals. A typical amplitude spectrum of a barometric pressure, with the exception of the tidal frequencies, reflects the rapidly decreasing energy content in the signal for the higher frequencies. In the time domain, this means that the higher frequencies will be represented by very small excursions from the much larger lower frequency signal associated with major weather changes. In the time domain inverse problem, these small excursions will play a much smaller role in influencing the solution since the solution convergence is governed by the square of the deviation of the model from the data. If the tidal bands were not potentially contaminated with thermal effects in the measurements, the problem would be less severe since there is a rather large energy content at these higher frequencies associated with the tides. However, it has been shown that, unless measures are taken to minimize or eliminate these thermal effects (see for example, Hanson, 1984), they should probably be eliminated prior to data analysis. To date, no such measures have been taken in barometric pressure transient testing at the Nevada Test Site.

If the analysis is carried out in the frequency domain, however, there are simple procedures available to force the higher frequencies of the signal to play a stronger role in influencing the solution. The easiest method, which will be discussed later, is simply to apply a larger weighting factor to these higher frequencies when calculating the rms deviation (ie. chi-square) of the model from the data (all in the frequency

domain).

On the less optimistic side of things, several problems may arise with frequency domain analysis which may preclude its use as a practical method. The first of these problems is associated with the nature of the diffusion equation itself. The subsurface pressure record depends upon the total history of the surface pressure record. Since the latter is not known, this may present a significant problem. For the case of time domain analysis, this problem is easily overcome by "running" the model for a given time period t^* and to let the computed pressure distribution at $t=t^*$ be the initial pressure distribution for the purpose of analysis. The problem of finite data sets for frequency domain analysis is less straightforward. The usefulness of using a product rather than a convolution may be outweighed by error introduced by the finiteness of the record length. This problem will be discussed later.

Another problem closely associated with the problem above has to do with the nature of the data itself. The barometric pressure record, particularly for the data lengths under consideration, cannot be considered a stationary signal. By stationary we mean that its frequency content is independent of time. The process of casting the surface and subsurface barometric signals in the frequency domain assume that the signals are repetitive in time. This is acceptable in dynamic systems that have reached steady state - for example, mechanical structures under a stationary sinusoidal loading history. Under these conditions, the transfer function can be precisely computed in the frequency domain. For diffusion processes, on the other hand, the computed transfer function is contaminated by our lack of knowledge of the total history of the surface load. The error introduced by this contamination is much less easily accounted for than by carrying out the analysis in the time domain.

As will be shown later, the analysis of barometric pressure records in the frequency domain can be forced to be equivalent in all respects to analysis in the time domain. However, by forcing the method to conform to the nature of the diffusion equation, the computation scheme in the frequency domain requires the evaluation of the system impulse response in the time domain, which negates our expectation of speeding up the computation time. The one situation in which the question of signal stationarity may be minimized is by carrying out the barometric analysis at the atmospheric tidal frequencies. At these frequencies, the signals can to good approximation be considered stationary, and spectral analysis techniques under these conditions and for finite length records are straightforward (Hanson, 1984). However, as has been shown previously (Hanson, 1984), the pressure signal at the tidal frequencies are often contaminated by temperature effects unless some effort is made in the data acquisition phase to minimize these effects.

The general form of the frequency response of a chimney-formation system is most easily derived by beginning in the time

domain. In the following, we will assume 1-D (vertical) flow. However, the conclusions are easily generalized to 2-D or 3-D flow situations. Recalling from equation (3-11) that, for an arbitrary surface pressure perturbation history $p(0,t)$, the subsurface response $p(z,t)$ is given by:

$$p(\vec{r},t) = \int_{-\infty}^t G(\vec{r},t-\tau) p_0(\tau) d\tau \quad (3-34)$$

where $G(\vec{r},t)$ is the impulse response of the system which contains all of the information regarding the geometry and gas flow properties of the system. We assume, for the purpose of discussion, that the surface pressure history $p(0,t)$ is a pure oscillation given by $p(0,t) = p_0 \exp(i\omega t)$, where ω is the angular frequency and where p_0 is the amplitude (absolute value) of $p(0,t)$. Equation (3-34) can, with some algebra, be shown to be equivalent to:

$$p(\vec{r},t) = p_0 e^{i\omega t} \tilde{G}(\vec{r},\omega) \quad (3-35)$$

where $\tilde{G}(\vec{r},\omega)$ is the one-sided Fourier transform of the time-domain impulse response, defined by:

$$\tilde{G}(\vec{r},\omega) = \int_0^{\infty} G(\vec{r},t) e^{-i\omega t} dt \quad (3-36)$$

There is a much easier way of calculating the frequency domain transfer function under the above stated conditions. This is simply to assume at the start that $p(\vec{r},t)$ can be represented in the form $p(\vec{r}) \times \exp(i\omega t)$ and solve the diffusion equation

directly. However, we underscore that this approach again presupposes that the total history of the surface pressure perturbation is known and that the frequency content is stationary, a situation that is unrealizable.

The following example for the infinite half-space problem describes the differences between the frequency domain transfer functions assuming that infinite or finite history surface pressure histories are available. Under the assumption that the surface pressure history is known for all time prior to time t , the frequency domain transfer function is calculated using equations (3-9) and (3-36):

$$\tilde{G}(z, \omega) = \int_0^{\infty} \frac{z}{2\sqrt{\pi c t^3}} e^{-\frac{z^2}{4ct}} e^{-i\omega t} dt \quad (3-37)$$

Carrying out the integration, it can be shown (Gradshteyn and Ryzhik, p. 340, #9) that:

$$\tilde{G}(z, \omega) = \frac{z}{\sqrt{\pi c}} \left(\frac{z^2}{4i\omega c} \right)^{-1/4} K_{-1/2} \left(z \sqrt{\frac{i\omega}{c}} \right) \quad (3-38)$$

where the solution is in terms of a modified Bessel function (of the second kind) of fractional order and with complex argument. This rather obscure result is clarified by the relationship (Gradshteyn and Ryzhik, p. 967, #8.469):

$$K_{-1/2} \left(z \sqrt{\frac{i\omega}{c}} \right) = \left(\frac{\pi}{2z} \right)^{1/2} \left(\frac{c}{i\omega} \right)^{1/4} e^{-z \sqrt{\frac{i\omega}{c}}} \quad (3-39)$$

which results in identifying:

$$p(z, t) = p_0 e^{i\omega t} \tilde{G}(z, \omega) \quad (3-40)$$

where:

$$\tilde{G}(z, \omega) = e^{-z \sqrt{\frac{i\omega}{c}}}$$

Thus for a given frequency ω , the system response is equal to the product of the Fourier transforms of the system input and the impulse response. This result is widely known. The reason it is again agonized over will become quite apparent when contrasted with the usual situation in which an infinite amount of data is NOT available. The result presented in eq. (3-40) is precisely the solution obtained had one began with the solution form $p(z, t) = p'(z) \times \exp(i\omega t)$ and solved the diffusion equation directly.

The following presents a parallel derivation of the subsurface pressure response under the more realistic case of an unknown pressure history prior to $t=0$ (our defined starting time for the pressure measurements). Using eq. (3-34) and a surface pressure of the form $p(0, t) = p_0 \exp(i\omega t)$, p_0 real, the general form for the subsurface pressure response is:

$$p(z, t) = p_0 \tilde{G}(z, \omega) + p_0 e^{i\omega t} \left\{ \int_0^t e^{-i\omega \xi} \tilde{G}(z, \xi) d\xi \right\} \quad (3-41)$$

The term on the left is simply a complex number (or equivalently amplitude and phase) which depends upon frequency, depth, and formation gas flow parameters. This term is the analog of the "initial formation pressure distribution" for time-domain models. This term is generally unknown and will serve to introduce a time-independent frequency-dependent offset in the complex domain. Looking at equation (3-40), one expects that the offset will be largest for small frequencies and/or large diffusivities. Unlike time-domain analysis, we cannot effectively eliminate this term by "running" the model for a period of time - it's independent of time.

If one is to define a frequency domain transfer function as "that function, when multiplied by the Fourier transform of the input, yields the Fourier transform of the output", then the frequency-domain transfer function is the expression in the brackets in equation (3-41). It is clearly seen that, for the practical situation of a finite-duration data set, the transfer function (in the frequency domain) is in general dependent on time! As a result, casting barometric pressure transient analysis in the frequency domain DOES NOT reduce the problem to a product - one of the primary reasons for considering frequency domain analysis to begin with. However, we point out that time-domain models described previously which use the concept of impulse response for arbitrary surface pressure histories can be (in principal) converted to frequency domain analysis through equation (3-41).

Finally, we note that for "large" t , the expression given in eq. (3-41) looks like eq. (3-40), which was derived assuming an infinite pressure history is available. The only difference is a time-independent offset. Thus, for "large" t , the system output may again be approximated by multiplying the Fourier transform of the system input with the Fourier transform of the (time-domain) impulse response. A quantification of "large" can be carried out by determining at what time t the remaining contribution of the integral in eq. (3-41), (i.e. the tail of the time-domain impulse response) is small. This value of t will be on the order of $t=t^*$, where t^* is the "equilibration time" introduced in the time-domain analysis discussion.

In terms of a practical approach to doing barometric testing analysis in the frequency domain for arbitrary 1-D, 2-D, or 3-D chimney-formation models, the following procedure is recommended:

- (a) for a given set of system gas flow parameters and sensor depth, calculate the impulse response in the time domain AND the frequency domain.
- (b) pick a frequency band (ω_1, ω_2) over which the system response is to be calculated.
- (c) calculate the system response on a frequency by frequency basis according to eq. (3-41), where $p_0 \exp(i\omega t)$ is replaced by the Fourier transform of the surface barometric signal.
- (d) if this is a forward model, your'e done!
- (e) if this is an inverse problem, compare frequency-domain system output with Fourier transform of measured output. Update parameters and go to (a).

In summary, the correct solution for the infinite half-space assuming that the pressure history prior to $t=0$ is unknown is given by equation (3-41). It is now clear that there will be an error introduced if one simply calculates the Fourier transform of the measured surface and downhole pressure histories and uses

the one-sided Fourier transform of the time-domain impulse response as the theoretical transfer function. This approach yields a frequency-domain transfer function that is independent of time. Equation (3-41) shows that if the pressure history is unknown for $t < 0$, the frequency-domain transfer function depends on time - i.e., the transfer function is non-stationary. For expediency, we have not at this time quantified the error introduced by assuming transfer function stationarity. Indeed, we have gone ahead, in spite of reservations associated with the above discussion, and used this approximation in the following and in Chapter IV. We suggest that more work be done to quantify problems associated with this approximation.

Frequency domain transfer functions have been derived for the chimney-formation models considered previously. The transfer functions are evaluated on the assumption that the total pressure history is known and therefore, that the transfer function (frequency domain) is independent of time (i.e. stationary). This is done principally for expedience and we point out that the use of these transfer functions must be done with the knowledge that some error will be introduced as discussed above. With this assumptions, the transfer functions are easily obtained by assuming a form $p(\vec{r}, z, t) = p'(\vec{r}, z) \times \exp(i\omega t)$ and solving the diffusion directly. An equivalent approach, which is used for the cylindrical chimney model, is to sum the residues of the Laplace space solutions, making the association $s = i\omega$ or $s = -i\omega$. We again emphasize that the frequency domain transfer functions are approximate from the standpoint that, for practical purposes, we do not know the history of the surface pressure prior to $t=0$. As a result, an error is introduced. The exact (time dependent) transfer functions should be derived or calculated numerically from equation (3-41).

Derivations of the frequency-domain transfer functions are not presented here. The derivations are straight-forward using techniques suggested above. Code modules FDCMOD1-FDCMOD4, when linked with DRIVER2, calculate the forward and inverse solutions to the frequency-domain uniform half-space and layered half-space situations.

3.2.2 Numerical Examples - Frequency Domain

Again, a comparison of the finite difference chimney model with the semi-analytic cylindrical chimney model was carried out. The geometry of the chimney-formation system used was the same as that given in section 3.1.8, with the exception that the no-flow boundary was taken to be $z=1000$ m. The permeability of the chimney and the permeability of the formation was assumed to be 10 Darcy. With this assumption, the frequency domain half-space model (with "no-flow" boundary) could be used for comparison with the numerical finite difference solution. We point out that we have not presented a semi-analytic frequency-domain solution for the cylindrical chimney model in this report. Such a solution is

obtained in a straight-forward manner by evaluating the residues of equation 3.33 at the poles $s=+i\omega$ and $s=-i\omega$. This procedure is discussed in Peavy (1968).

The number of vertical nodes between the surface and the sensor and between the sensor and the no-flow boundary, and the number of radial nodes in the chimney, were also the same as in section 3.1.8. The convergence criterion for the alternating direction finite difference solution was again taken to be 1 Pa. In all cases, the surface pressure variation was taken to be $p(0,t) = p_0 \exp(i\omega t)$, where the surface pressure amplitude p_0 was taken to be unity.

The numerical finite difference calculations were done using code modules RCHAN and FCHAN. The semi-analytic solution was carried out using the code module FDCMOD3, where the vertical averaging distance was taken to be small. Listings of these programs are given in Appendix I.

Figures 3.8 and 3.9 show the pressure amplitude and phase of the downhole pressure variation for both the numerical solution and the semi-analytic solution, respectively. Figures 3.10 and 3.11 show the real and imaginary parts of these respective solutions. There is reasonable correspondence between the semi-analytic and numerical solutions indicating both are calculating the same solution. We point out that the inflection in the phase shift is not real but an artifact introduced by the arctangent function used for the calculation of phase.

A second numerical example was carried out assuming that a chimney of 50 m. radius and 100 m. depth was embedded in a uniform finite half-space of 500 m. depth. A no-flow boundary was placed at depth 500 m. A total of 40 vertical nodes were used, 20 of which spanned the depth of the chimney, the remainder below the chimney. Ten radial nodes were used within the chimney and the outer (no-flow) radius was taken to be 1 km. The formation and chimney porosities were taken to be 0.2. The formation permeability was taken to be 10 Darcy. Five cases were considered corresponding to 5 chimney permeabilities: 1 Darcy, 5 Darcies, 10 Darcies, 20 Darcies, and 100 Darcies. Figures 3.12 and 3.13 show the amplitude and phase, respectively, for these five chimney permeability cases. Figures 3.14 and 3.15 show the real and imaginary parts, respectively, of the five cases.

Figure 3.8. Comparison of amplitude spectra for numerical (solid) and analytic (dashed) cylindrical chimney models.

Figure 3.9. Comparison of phase spectra for numerical (solid) and analytic (dashed) cylindrical chimney models.

Figure 3.10. Comparison of real spectra for numerical (solid) and analytic (dashed) cylindrical chimney models.

Figure 3.11. Comparison of imaginary spectra for numerical (solid) and analytic (dashed) cylindrical chimney models.

Figure 3.12. Amplitude spectra for five chimney-formation systems (cases are discussed in text).

Figure 3.13. Phase spectra for five chimney-formation systems (cases are discussed in text).

Figure 3.14 Real spectra for five chimney-formation systems (cases are discussed in text).

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Figure 3.15. Imaginary spectra for five chimney-formation systems (cases are discussed in text).

CHAPTER IV

INTERPRETATION OF HISTORIC AND RECENT CHIMNEY DATA IN TERMS OF HALF-SPACE AND MULTI-LAYER MODELS

The following presents the interpretation of barometric pressure transient data taken on nuclear chimneys. The models used in the interpretations have been described in the previous chapter. This chapter is broken down into several sections. The first section discusses the method of inversion used to carry out the data interpretation and restrictions on interpretation due to the nature of the slant-hole access port. This section is followed by sections on: (1) time-domain reinterpretation of the historic chimney data and validation of previously published values of gas flow parameters in these chimneys and (2) a time-domain interpretation of recently acquired chimney data at U2fe, U2ff, U2ev, and U19ac. In the latter, the differences between pre- and post-shot diffusivity at U2fe and U19ac are discussed.

This is followed by sections describing an equivalent frequency-domain analysis of (1) historic chimney data and (2) recent chimney data. The next section evaluates the modification of calculated diffusivity should all tidal constituents be removed to eliminate any possibility of thermal contamination of the signal. This was done for both time- and frequency-domain analysis and for both historic and recent chimney data.

To this point, all interpretations have assumed a homogeneous and isotropic half-space. The chapter concludes with a section on multi-layer models of recent chimney data. These interpretations are carried out in the frequency-domain and validated by forward models in the time-domain.

4.1 Data Interpretation Methods and Data Quality

Chimney models presented in the last chapter were used to interpret barometric pressure data taken historically and more recently. The historic data includes chimneys designated DH3, DH5, DH6, DH7, and DH9. The more recent data includes chimneys U2fe, U2ff, U2ev, and U19ac.

The general procedure for determining estimates of the gas flow parameters for the chimney and formation is to adjust these parameters in the model until a "best fit" is obtained between the subsurface pressure perturbation predicted by the model and the measured subsurface pressure data. The adjustment of parameters can be carried out using a variety of non-linear least squares methods: grid searching methods, ridge regression, and monte carlo. These non-linear least squares

techniques are explained in more detail in Hanson (1984) and Bevington (1969). Although slower than the ridge regression method, the grid searching technique offers more stability and therefore was used in all of the following inverse problems.

As was discussed in Chapter II, the historic subsurface chimney data was taken through a perforated tube grouted into a partially cased hole. This resulted in an effective, spatially-limited access port over which subsurface pressure was measured. The data was taken via tubing from the subsurface port to the surface, where a sensor measured the pressure. There was typically a significant distance between the surface casing and the pressure sensor over which the tubing was subject to surface temperature variations corresponding to the 24 hour thermal cycle. This variation in temperature can give rise to a pressure variation and is discussed in some detail in Hanson (1984). The presence of this contamination will be shown conclusively, in a later section, by comparing the predicted subsurface pressure with the measured subsurface pressure for given model. Figures 4.2 and 4.7, for chimneys DH5 and U2ff, respectively, show the presence of 24 hour thermal contamination. One can remove this contamination by appropriate spectral analysis techniques, to be discussed later. However, in doing so, one runs the risk of eliminating higher-frequency information which may be necessary to constrain the model solution. A better solution to this problem is to simply take a few simple precautions, in terms of insulation or temperature compensation, prior to data acquisition.

The existence of a large open hole section complicates data interpretation for the recent chimney data taken on U2fe, U19ac, U2ev, and U2ff. First, as was pointed out by Hanson (1984), the open hole section serves to average the effects of the different gas flow properties of the adjacent formation. This in turn creates a rather ill-posed inverse problem when trying to identify these different gas flow properties. Secondly, since the observation holes are not situated on the axis of the chimney, radial symmetry is broken. As a result, axisymmetric chimney models are no longer valid. This observation is based on the fact that a large open hole section will perturb the flow geometry significantly (Hanson, 1984). Had the slant holes been stemmed with the observation port limited in spatial extent, the symmetry would have been restored.

It is our understanding that cost was the primary consideration in leaving the hole below the casing open rather than isolating the subsurface sensor with stemming material in the slant holes (personal communication, Dr. Joseph Hearst, LLNL). This decision clearly has impact in two areas: (1) the degree of model sophistication warranted in subsequent data analyses and (2) the general establishment of the barometric pressure transient technique for determining subsurface gas flow parameters for situations other than "trivial" (i.e. the assumption of a homogeneous and isotropic half-space).

Due to the nature of the data acquisition, we feel that the only chimney models that can rationally be justified in interpreting the recently acquired chimney data (U2fe, U2ff, U2ev, and U19ac) are the 1-D vertically averaged chimney model and the 1-D (vertical) layered half-space model. This statement is of course subject to the caveat that, budget permitting, one could indeed use a full 3-D numerical model to interpret the data. This degree of modelling effort is beyond the scope of the current project. We suggest here that, given the options of: (1) grouting the slant hole to limit the spatial extent of the observation port and using 1-D or 2-D models for interpretation or (2) leaving the uncased part of the slant hole open and using a full 3-D numerical model for interpretation, option (1) will clearly be more cost effective in the long term and will likely yield more believable results.

4.2 Interpretation of Historic Chimney Data - Time Domain

The barometric pressure data for chimneys DH3, DH5, DH6, DH7, and DH9 which were presented in chapter II were reanalyzed in terms of the 1-D (vertical) flow chimney models described in previous chapter. This is an infinite half-space model that does not take into consideration a no-flow boundary (eg. water table) at depth. The code modules used in the interpretation "DRIVER2" linked with "TDCMOD1". Both modules are given in Appendix I. Table 4.1 summarizes the results obtained using the infinite half-space model.

TABLE 4.1

Reinterpretation of Historic Chimney Data;
(Time Domain, Infinite Half-space)

Chimney	Sensor Depth (m)	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
DH3	165	2474	52	33
DH5	216	468	5	6
DH6	340	2827	63	37
DH7	220	360	1	5
DH9	270	2021	22	28

Permeabilities listed in Table 4.1 were computed assuming a connected porosity of 20%, a mean static pressure of 85 kPa, and a gas viscosity of 0.00002 Pa-sec. Uncertainties in the computed diffusivity are at the 1-sigma level. These results are generally consistent with the earlier analyses of these chimneys (see Table 2.1). However, the discrepancies are statistically significant at a 99% confidence level. These discrepancies may be a result of the fact that earlier analyses, for the most part, relied on the subjective "visual" least squares fit rather than on the less subjective method of realizing a quantitative least squares criterion.

Figures 4.1 - 4.5 show the best fit of the homogeneous and isotropic half-space model to the data. Only the variation from the mean static pressure, for both measured and predicted pressure, is shown in these figures. The mean static pressure was assumed to be 85 kPa in all cases.

The historic data was not analyzed in terms of more complex models due to the fact that sufficient information regarding location of the water table, lithology (ie. stratigraphic breaks), and chimney geometry was unavailable.

4.3 Interpretation of Recent Chimney Data - Time Domain

During 1984 and 1985, barometric pressure transient data from four more nuclear chimneys at the NTS were taken. In the following, the chimneys are designated by their respective emplacement holes. Three of the chimneys are in Area 2: U2ev, U2ff, and U2fa. The fourth chimney is located in Area 19 on Pahute Mesa: U19ac. Chapter II describes in detail the geologic and structural setting of each of these sites. Unlike earlier chimney pressure measurements which restricted the measurement port to a small spatial volume by stemming the hole from the port to the surface, current measurements left the hole open from the bottom of the casing to the bottom of the hole. In some cases, this open section accounted for a large fraction of the total hole depth. Table 4.2 shows casing, hole, and water table depths as well as estimated chimney radii and chimney depths (personal communication, Dr. Joseph Hearst, LLNL).

Figure 4.1. Measured (solid) and predicted (dashed) downhole pressure for DH3. Infinite half-space, 1-D (vertical) model.

Figure 4.2. Measured (solid) and predicted (dashed) downhole pressure for DHS. Infinite half-space, 1-D (vertical) model.

Figure 4.3. Measured (solid) and predicted (dashed) downhole pressure for DH6. Infinite half-space, 1-D (vertical) model.

Figure 4.4. Measured (solid) and predicted (dashed) downhole pressure for DH7. Infinite half-space, 1-D (vertical) model.

Figure 4.5. Measured (solid) and predicted (dashed) downhole pressure for DN9. Infinite half-space, 1-D (vertical) model.

TABLE 4.2

Chimney-Formation Geometry at U2ev, U2ff,
U2fe, and U19ac

Chimney	Chimney Radius (m)	Chimney Depth (m)	Water Table (m)	Casing Length (m)	Hole Length (m)
U2ev	38.5	358	579	117	313
U2ff	38.1	364	569	201	321
U2fe	47.4	437	579	33	494
U19ac	54.7	605	696	387	632

Chimney data from U2fe, U19ac, U2ff, and U2ev were analyzed in terms of the 1-D vertically averaged model. Hanson (1984) has shown that this model is an excellent approximation to the more rigorous 2-D (radial and vertical) gas flow model, assuming the formation is homogeneous and isotropic. Again, this model assumes that the gas flow properties, namely permeability and diffusivity, are the same for chimney and adjacent formation. It also assumes that both are homogeneous and isotropic and that there are no "no flow" boundaries to flow with depth. The code modules "TDCMOD3", linked with "DRIVER1", both given in the appendix, were used in these calculations. Table 4.3 presents the results of applying this model to the above data.

TABLE 4.3

Analysis of Chimney Data (Time Domain - V.A.)
U2fe, U19ac, U2ff, and U2ev

Chimney	Hydraulic Diffusivity (m ² /hr)	Uncertainty (1-sigma) (m ² /hr)	Data Matching Interval (hrs)
U2fe	9370	189	100 - 500
U19ac	3599	102	150 - 500
U2ff	188	5	200 - 400
U2ev	2288	63	100 - 500

Figures 4.6 through 4.9 show the best fit model superimposed on the measured data, respectively. Again, only the deviation from the mean static pressure (assumed 85 kPa) is shown.

Of particular interest are the values of hydraulic diffusivity for U2fe and U19ac. Barometric testing has been carried out on

Figure 4.6. Measured (solid) and predicted (dashed) downhole pressure for U2fe. Infinite half-space, 1-D (vertical average) model.

Figure 4.7. Measured (solid) and predicted (dashed) downhole pressure for U2ff. Infinite half-space, 1-D (vertical average) model.

Figure 4.8. Measured (solid) and predicted (dashed) downhole pressure for U2ev. Infinite half-space, 1-D (vertical average) model.

Figure 4.9. Measured (solid) and predicted (dashed) downhole pressure for U19ac. Infinite half-space, 1-D (vertical average) model.

these holes prior to the shot and analyzed by Hanson (1984). The interpretation model used in the latter assumed a partially cased, but otherwise open, hole within which the "in-hole" pressure measurement was taken. In other words, the interpretation model used was identical to the model used in the chimney data analysis tabulated above. Tables 4.4 and 4.5 give the results of the open hole analysis for U19ac and U2fe, respectively, using this model.

TABLE 4.4

Pre-Shot Open Hole Analysis at U19ac
(from Hanson, 1984)

Date Set	Hydraulic Diffusivity (m**2/hr)	Uncertainty (1-sigma) (m**2/hr)	Permeability (Darcy)
#1	91640	4134	60
#2	51280	3120	34
#3	58700	2035	38
#4	50530	1623	33
#5	22710	675	15

Permeability was calculated assuming a connected porosity of 0.01. This value, although small in terms of porosity of sedimentary formations, is of the proper magnitude (or even slightly high) for fractured volcanics (Snow, 1968).

The overall decrease of hydraulic diffusivity at U19ac indicated in Table 4.4 was attributed to increasing precipitation levels which resulted in pore space blockage near the surface (Hanson, 1984). The bottom of the casing (surface conductor) was at a depth of 17.7 m and the bottom of the emplacement hole was at 701 m. It is appropriate here, for the purposes of discussion later, to point out the significantly different casing depths for pre-shot (17.7 m.) and post-shot (387 m.) data acquisition at U19ac.

TABLE 4.5

Pre-shot Open hole analysis at U2fe
(from Hanson, 1984)

Hydraulic Diffusivity (m**2/hr)	Uncertainty (1-sigma) (m**2/hr)	Permeability (Darcy)
4806	117	30

The casing depth for pre-shot and post-shot data acquisition at U2fe are essentially identical (33 m.). The calculation of permeability assumed a connected porosity of 0.093. The calculated permeability assumes a connected porosity of 0.2.

It is clear from the above that there is a considerable difference in diffusivity between pre- and post-shot at both U2fe and U19ac. For the case of U2fe, there is a factor of two increase in diffusivity. U19ac shows a factor of 25 decrease. There are several possible explanations for this behavior.

For the case of U2fe, the increase in diffusivity may be attributed to (1) a decrease in connected porosity due to compaction near the shot point or (2) an increase in permeability further away from the shot point due to the shock loading of the formation. Either of these mechanisms (or possibly both) can be expected at U2fe, which is completed in a sediment. One expects a considerable degree of compaction in sediments due to the magnitude of the load placed on the formation near the shot. However, surface effect maps for the alluvial regions of the NTS suggest that permeability enhancement, in the form of pervasive fracturing, can occur at significant distances from the shot point. In either case, the factor of two increase in diffusivity from pre- to post-shot at U2fe should not be considered large.

On the other hand, the factor of 25 decrease in diffusivity from pre- to post-shot observed at U19ac is probably due to a combination of (1) differences in casing length and (2) simplicity of the half-space model. The large diffusivity calculated pre-shot at U19ac on the open hole analysis is probably a consequence of a high diffusivity upper stratigraphic horizon underlain by less permeable formations. If this is the case, the observed pre- to post-shot reduction in diffusivity observed at U19ac does not necessarily reflect a change in diffusivity near the shot point. It is more likely that the change reflects the different depth at which the hole was open to the formation (ie. different casing depths for pre- and post-shot data acquisition).

Two observations give credibility to this argument. The first is that, for the pre-shot open hole analysis, the casing ("surface conductor") length was 18 m, the remainder of the hole being open. For the post-shot data, the hole was cased to 387 m., the remainder of the hole being open. If the formation below 387 m. has a diffusivity considerably less than that for the region between the surface and 387 m, the inferred diffusivity from the barometric pressure tests may be more strongly influenced by this "tighter" formation than if the casing length were on the order of tens of meters. At U19ac, a depth of 387 m. corresponds very closely with the transition from the Timber Mountain formation and the Paintbrush tuff. The former consists principally of vitric ash-flow tuffs and the latter principally of ash-fall and reworked bedded tuffs. Vitric tuffs have been shown to have, through air injection tests, a much higher permeability than ashfall tuffs (Snoeberger, et al., 1971).

Another observation that lends support to the hypothesis that the large inferred pre-shot diffusivity at U19ac is due to a high diffusivity in an upper horizon is from a multi-layer analysis of the pre-shot open-hole data. Using a multi-layer model for U19ac consisting of three layers corresponding to the Timber Mountain tuff, the Paintbrush tuff, and underlying rhyolite lava flows, Hanson (1984) found that the Timber Mountain tuff (0 - 395 m) exhibited a permeability several times higher than underlying formations. In spite of the ill-posed nature of the multi-layer open-hole analysis, this method did indeed reflect a higher permeability near surface layer. Table 4.6 shows the inferred permeability of the three principle horizons intersected by U19ac.

TABLE 4.6

Inferred Permeabilities on Open-hole Pre-shot U19ac
Using Data Set #4
(from Hanson, 1984)

Depth Interval (meters)	Stratigraphic Unit or lithology	Permeability (darcies)
0 - 395	Timber Mountain Tuff	44.5
395 - 530	Paintbrush Tuff	13.4
530 -	Rhyolite lava	22.0

The results shown in Table 4.6 assume a formation connected porosity of 0.01.

The value of permeability in the upper horizon (Timber Mountain Tuff) from Table 4.6 can be translated to a diffusivity of 67,195 m²/hr. This value is not significantly different in magnitude from that computed using a simpler half-space model (see Table 4.4, data set #4). This suggests that the simple half-space model is dominated by the diffusivity of the stratigraphic horizon nearest the surface in which there exists a section of open (uncased) hole.

The actual frequency content of the surface barometric pressure signal in itself has much to do with the ability of the barometric pressure transient method to detect horizons of high or low permeability. Most of the energy in the barometric signal is at the lower frequencies corresponding to periods greater than 40 hours. As a result, fitting a model to observed barometric data will tend to give more weight to the low frequency content of the signal. A high permeability horizon near the surface (or anywhere in the half-space, for that matter) will be given less weight in fitting a model since such an horizon will significantly alter the subsurface pressure signals only at higher frequencies. If we are dealing with a layered half-space in which the subsurface sensor is isolated as a point measurement (as opposed to an open hole situation), the inverse model will be influenced most strongly by the "tightest" horizon (or horizons) between the surface and the sensor. For an open-hole type of analysis, in which the down-hole sensor is suspended in an open hole intersecting several formation types, the situation is somewhat different. In this case, the characteristics of the near surface horizon will influence the inverse solution the greatest if there is a section of uncased hole within this horizon.

If the energy density of the barometric pressure signal were uniformly distributed in frequency (eg. white noise), these problems would in principal be minimized. However, Nature clearly does not conform to this ideal situation. Also, from a practical standpoint, time domain analysis would be difficult if the surface barometric pressure signal was white noise. Frequency-domain analysis would be much more appropriate for this situation (see for example, Goldman, 1968). However, there are several methods available to us to improve the situation over the hand that Nature has dealt us. The technique we have chosen in the following is to carry out the analysis in the frequency domain. Chapter III discusses this technique in some detail. As was pointed out, there are some subtleties associated with frequency domain analysis as a consequence of memory associated with diffusion processes. Some care must therefore be taken to account for the fact that we do not have available an infinite surface and downhole pressure history record.

For time-domain analysis, it is a simple matter to allow the model to "equilibrate" over a given period of time before we try to match a predicted pressure from a model to the measured pressure. In essence, this procedure allows us to approximate the "infinite pressure history" with a short segment of the data at the start of the recording. For "typical NTS permeabilities",

this can be made a reasonable approximation.

This is a straight-forward procedure in the time domain, but as discussed in Chapter III, is a much less straight-forward procedure for frequency domain analysis. In the latter, the theoretical amplitude and phase spectra predicted from a finite-length pressure record will depend on the time from the beginning of the record (see eq. 3-41) - that is, the theoretical spectra will be non-stationary, at least until the subsurface pressure has "equilibrated" with the surface pressure. After this time, the spectra will be stationary. However, it is no easy matter to calculate a time-dependent spectrum from a data record. The latter is required for data-matching procedures, either forward or inverse, in the frequency-domain. From a practical standpoint, therefore, one will probably have to carry out the frequency-domain analysis in the time-domain using equation (3-41) as a guide.

In the following, we have simply ignored the equilibration time problem in the frequency domain analysis. This was done due to computational time restrictions (see Chapter III) associated with complete frequency-domain analysis. The effects of this approximation have not been quantified in any rigorous fashion. However, comparisons with time-domain analysis results on both half-space and multi-layer models, as presented in the following, suggest that this approximation may not be as bad as one might expect.

4.4. Interpretation of Historic Chimney Data - Frequency Domain

A vertically averaged (V.A.), frequency-domain half-space chimney model was applied to the historic chimney data taken on chimneys DH3, DH5, DH6, DH7, and DH9. On this model, a partially cased but otherwise open hole is completed in a homogeneous and isotropic half-space. It is clear that the introduction of a non-zero length of open hole will introduce radial pressure gradients in the formation, requiring a 2-D formulation to adequately account for the vertical and radial variations in pressure. However, Hanson (1984) showed that the average of a purely 1-D (vertical) diffusion model over the open-hole (uncased) section yields a very good approximation to the 2-D flow situation, and is much more computationally efficient. Program module "FDCMOD1" linked with "DRIVER2" were used carry out the following inverse problems. These programs are given in Appendix I.

Since the "in-hole" data was, for these chimneys, taken on isolated point locations (ie. there was no significant open-hole sections), the length of the sensing hole was taken to only slightly longer (a few meters) than the casing length. This effectively forces a point response in the model. Table 4.7 gives

the computed values of diffusivity using this model. The amplitude spectra used contained all information on the 0 to 0.2 cph band. 200 values of spectral amplitude were used in the analysis. Sensor depths are given in Table 4.1.

TABLE 4.7

Calculated Diffusivities on Historic Chimney Data
(Frequency Domain)

Chimney	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
DH3	2190	106	29
DH5	902	37	12
DH6	3815	n/a	51
DH7	344	11	5
DH9	2594	208	36

Again, the permeability was computed assuming that the open connected porosity (for sediments) was 0.2 and a mean static pressure of 85 kPa. Generally, these results follow those computed on the bases of time-domain analysis which are presented in Table 4.1. There are, however, differences between these results and those obtained in the time domain which we attribute primarily to the assumption of stationary spectra and heating contamination of the pressure data. The latter is probably the principal cause for the difference between computed diffusivities for DH5, judging by the amount of thermal contamination of the signals (see Fig. 4.2). However, it is unclear why there is such a large difference in diffusivities for DH6. The spectra for DH6 (see Figs. 2.9a,b) look particularly noisy - this may have something to do with the problem.

4.5 Interpretation of Recent Chimney Data - Frequency Domain

An identical analysis was carried out on the more recent chimney data taken at U2fe, U2ff, U2ev, and U19ac. In these cases, the open hole section accounted for a rather large fraction of the total hole depth. Again, the vertical average of the 1-D (vertical) half-space model, in the frequency domain, was used in the analysis. The vertical average was taken over the distance from the bottom of the casing to the bottom of the hole. Table 4.8 shows the results of these analyses.

TABLE 4.8

Calculated Diffusivities on Recent Chimney Data
(Frequency Domain)

Chimney	Diffusivity (m ² /hr)	Uncertainty (m ² /hr)	Permeability (Darcies)
U2fe	8046	360	107
U2ff	118	13	2
U2ev	2092	58	28
U19ac	28580	4374	19

For calculating permeability in the above table, a connected porosity of 0.2 was assumed for U2fe, U2ff, and U2ev, which intersect primarily sedimentary formations. A connected porosity of 0.01 was assumed for U19ac, which intersects volcanics.

With the exception of U19ac, the above computed values of diffusivity generally follow those computed using time-domain analysis (see Table 4.3). The large value of diffusivity calculated for U19ac is likely a consequence that the higher signal frequencies have a larger weight in controlling the solution than they have in the time domain. The amplitude spectra are by definition positive functions whereas destructive interference due different signal phases can serve to decrease signal amplitudes in the time domain. Thus, if a high frequency component exists in the signal (eg. a tidal signal), it will probably have more influence in a frequency-domain analysis than in a time-domain analysis. With a larger weight, the inverse solution will be more sensitive to a higher permeability in the near surface horizon (if such exists), as discussed earlier. This hypothesis is confirmed in a later section.

4.6 Time and Frequency Domain Analyses - Tidal Frequencies Removed.

As was shown by Hanson (1984), diurnal heating effects can significantly perturb the surface and in-hole pressure measurements. This perturbation is independent of the gas flow properties of the formation and can therefore be considered noise contamination as regards pressure diffusion modelling. This contamination may influence the interpretation of the data in terms of either modifying the value of or increasing the uncertainty in the computed formation parameters. No attempt to remove or minimize this temperature contamination was carried out in the previously presented chimney barometric pressure data,

both historic and recent.

To a good approximation, the major component of temperature contamination will occur at the tidal frequencies associated with the solar tides (see Hanson, 1984). Removal of all information at these specific frequencies will, in principal, eliminate the thermal noise. It should be recognized that this procedure may also eliminate useful information at the higher frequencies which may be needed to constrain more sophisticated models (eg. multi-layer).

In spite of this reservation, a line spectral analysis was carried out on all of the data to eliminate all information at the principal tidal frequencies. Briefly, the procedure involves calculating a trend function consisting of frequencies below the minimum principal tidal frequency (0.04 cph) and subtracting this function from the original data. A least squares best estimate of the amplitudes and phases of the principal tidal components is then calculated using this resulting signal. This technique, referred to as "line spectral analysis" is discussed in detail in Hanson (1984). The best estimate of the tidal component is then subtracted from the original data to yield a signal which is, in the least squares sense, free of all information at the tidal frequencies.

Figures 4.10 - 4.14 show the surface and downhole data, with the tidal component removed, for historic chimney data at DH3, DH5, DH6, DH7, and DH9, respectively. Figures 4.15 - 4.18 show the surface and downhole data, with the tidal component removed, for chimneys U2fe, U2ff, U2ev, and U19ac, respectively. This information was Fourier transformed to obtain amplitude spectra for the surface and downhole pressure signals. Figures 4.19 - 4.23 show the amplitude spectra of the surface and downhole pressure signals for historic chimney data at DH3, DH5, DH6, DH7, and DH9, respectively. Figures 4.24 - 4.27 show the amplitude spectra of the surface and downhole pressure signals for chimney data at U2fe, U2ff, U2ev, and U19ac, respectively.

4.6.1 Interpretation of Historic Data - Time and Frequency Domains (Tidal Constituents Removed)

Tables 4.9 and 4.10 show the computed results for historic data on DH3, DH5, DH6, DH7, and DH9, where the tidal frequency component of the surface and downhole signals has been removed using the method discussed above.

Figure 4.10. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - DH3.

Figure 4.11. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - DHS.

Figure 4.12. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - DM6.

Figure 4.13. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - DH7.

Figure 4.14. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - DH9.

Figure 4.15. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - U2Fe.

Figure 4.16. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - U2ff.

Figure 4.17. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - U2ev.

Figure 4.18. Measured surface (solid) and downhole (dashed) pressure data after removal of all tidal components - U19ac.

Figure 4.19. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - DH3.

Figure 4.20. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - DH5.

Figure 4.21. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - DH6.

Figure 4.22. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - DH7.

Figure 4.23. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - DH9.

Figure 4.24. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - U2fe.

Figure 4.25. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - U2ff.

Figure 4.26. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - U2ev.

Figure 4.27. Surface (solid) and downhole (dashed) amplitude spectra after removal of all tidal components - U19ac.

TABLE 4.9

Calculated Diffusivities on Historic Chimney Data
(Time Domain, Tides Removed)

Chimney	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
DH3	3440	140	46
DH5	403	0.5	5
DH6	2578	50	34
DH7	403	10	5
DH9	3519	115	47

These values generally follow the results shown in Table 4.1, which were calculated in the time-domain but prior to removal of the tidal components. There are some significant differences, however, and without a more detailed investigation, we are not in a position to identify the precise origin of these differences. We expect, however, that the differences are due principally to signal contamination by heating.

TABLE 4.10

Calculated Diffusivities on Historic Chimney Data
(Frequency Domain, Tides Removed)

Chimney	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
DH3	2628	165	35
DH5	1139	75	15
DH6	4333	423	57
DH7	473	39	6
DH9	2011	138	27

The diffusivity values listed in Table 4.10 are similar to those values computed in the frequency domain prior to removal of the tidal constituents (Table 4.7).

4.6.2 Interpretation of Recent Chimney Data -
Time and Frequency Domains
(Tidal Constituents Removed)

Tables 4.11 and 4.12 show the computed results for recent data on U2fe, U2ff, U2ev, and U19ac, where the tidal frequency component of the surface and downhole signals has been removed using the method discussed above.

TABLE 4.11

Calculated Diffusivities on Recent Chimney Data
(Time Domain, Tides Removed)

Chimney	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
U2fe	9739	189	130
U2ff	207	4	3
U2ev	2286	28	30
U19ac	3754	110	2.5

These values compare very well with the time domain analysis results computed prior to the removal of all tidal constituents (see Table 4.3).

TABLE 4.12

Calculated Diffusivities on Recent Chimney Data
(Frequency Domain, Tides Removed)

Chimney	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)	Permeability (Darcies)
U2fe	9721	638	130
U2ff	275	5	4
U2ev	2018	78	30
U19ac	28070	3529	19

These results compare very well with the frequency-domain analysis result computed prior to the removal of all tidal constituents.

In calculating permeabilities in Tables 4.9 - 4.11, we have assumed a connected porosity of 0.2 for all of the chimneys with the exception of U19ac. The later, intersecting volcanics, was assumed to have a connected porosity of 0.01.

It is again clear, comparing the diffusivities computed for U19ac (Tables 4.11 and 4.12) that insufficient weighting is being given to the higher frequency components (in this case, of non-tidal origin) in the time-domain analysis. Because of this, the inverse solution in the time-domain is almost blind to the high-diffusivity near surface horizon (Timber Mountain Tuff) since this horizon will modify only that part of the signal at the higher frequencies. The lowest diffusivity in the vertical section (Paintbrush Tuff) will therefore influence most the effective diffusivity for the half-space. However, an amplitude spectrum gives more weight to the higher frequencies, thus making the near-surface high-diffusivity horizon again visible which results in a higher computed diffusivity for the half-space.

This proposition is confirmed by the following. We took the amplitude spectra data (after removal of tidal constituents) for U19ac and carried out a set of data interpretations, each weighting a separate frequency band. The weighting factor was taken to be 1000 - thus, all other frequencies in the 0.0 - 0.1 cph spectra would have insignificant influence on the inverse solution. The frequency-domain 1-D V.A. model was used in the interpretation. Table 4.13 shows the results.

TABLE 4.13

Calculated Diffusivities at U19ac (Frequency-Domain)
for Several Different Frequency Bands

Frequency Band (cph)	Diffusivity (m**2/hr)	Uncertainty (m**2/hr)
0.0 - 0.001	2396	164
0.0 - 0.005	14222	1358
0.0 - 0.015	22140	2223
0.0 - 0.025	24530	2723
0.0 - 0.035	26000	3036
0.0 - 0.050	26900	3222
0.0 - 0.100	28580	4374

As the high frequency component of the data is increased, the half-space model reflects more and more the high diffusivity associated with the near-surface horizon (Timber Mountain Tuff). However, at the lower frequencies, this high-diffusivity horizon is almost "invisible" (i.e. does not significantly perturb the subsurface pressure) and therefore does not significantly influence the inverse solution.

4.7 Multi-Layer Models - Recent Chimney Data

In order to properly carry out a multi-layer modelling effort on the recently acquired chimney data at U2fe, U2ff, U2ev, and U19ac, one should use a full 3-D chimney-formation numerical model. The dimensionality of the model is prescribed by the fact that a large section of open (uncased) hole was left in the slant hole access ports. As shown by Hanson (1984), an open-hole section can induce significant radial pressure gradients, requiring the use of a model that can account for both vertical and radial pressure variations. This is true in all cases but the homogeneous and isotropic half-space, in which the vertical average 1-D model can effectively represent the more complicated 2-D situation. For the case under consideration, even a 2-D model would be insufficient since the slant holes are not axisymmetric on the chimney-formation system, destroying any possibility of cylindrical symmetry in the model. Unfortunately, a 3-D modelling effort is beyond both the scope and budget of this project.

We have therefore (with some reservations) interpreted the recently acquired chimney data in terms of the layered half-space model. This model assumes that the gas flow properties of the chimney are identical to the formation on a depth-by-depth basis, although a vertical distribution of permeability and/or porosity is allowed. The following present the results of the multi-layer models. It is recommended that the limitations of the model as regards its representation of a chimney-formation system always be kept in mind.

Multi-layer models on the historic chimney data were not carried out due to the lack of information on lithology and stratigraphic breaks at each of the sites.

Four different cases were used in analyzing the chimney data in the frequency domain:

- Case "A" - Amplitude spectra with all tidal components retained.
No enhanced weighting of the higher frequencies.
- Case "B" - Amplitude spectra with all tidal components retained.
Enhancement of weight applied to higher frequencies.
- Case "C" - Amplitude spectra with all tidal components removed.
No enhanced weighting of the higher frequencies.
- Case "D" - Amplitude spectra with all tidal components removed.
Enhancement of weight applied to higher frequencies.

The frequency weighting referred to in the above is simply that, in the inverse problem, in which the measure of "goodness-of-fit" is the rms deviation (chi-square) of the model from the data, a given frequency band is weighted by a constant factor greater than 1. Normally, the higher frequencies in a barometric pressure record have amplitudes significantly smaller than the lower frequencies associated with long-period weather changes. Using the modified weighting scheme, the higher frequencies in a barometric pressure spectrum can be given as much weight as the lower frequencies. Table 4.13 shows the weighted frequency bands and the weighting factor used for Cases "B" and "D".

TABLE 4.14

Weighted Frequency Bands and Weighting Factors

Chimney	F (low) (cph)	F (high) (cph)	Weight
U2fe	0.02	0.1	3
U2ff	0.01	0.04	4
U2ev	0.02	0.1	5
U19ac	0.02	0.1	5

The smaller value of F (high) used for U2ff was due to the fact that this chimney exhibited very small diffusivity, and thus the spectrum fell off rapidly with increasing frequency. It was felt that to weight frequencies any higher than 0.04 cph would be effectively be weighting noise.

Figures 4.28 - 4.31 show the multi-layer results for U2fe for the four cases listed above, respectively. In these and all of the following multi-layer models, the position of the sensor was chosen to be the mid-point of the open hole section. One could of course done a vertical average of the solution over the open hole. However, Hanson (1984) has shown that this approximation can be very poor for multi-layer systems. In light of all of the other approximations used, our choice of midpoint location seemed both prudent and conservative.

It is interesting to note that, for both cases "A" and "B", the upper layer permeability of 36 Darcies is exactly that computed pre-shot for the same layer and using multi-layer time-domain analysis (Hanson, 1984, p. 67). The latter analysis used a full 2-D numerical solution. The lower horizon yielded a permeability of 23 Darcies, a factor of one-half that for the pre-shot analysis. Note that the porosities used in the current analysis are the same as those used by Hanson (1984) for the pre-shot analysis.

Removal of the tidal constituents greatly modified the results, as shown by Figures 4.30 and 4.31. In both cases, the computed permeabilities for both horizons were significantly larger, and in both cases, the inversion run had to be terminated prior to convergence. In this case, it would seem that the tidal constituents represented the only "non-noise" higher frequency components and eliminating them also eliminated necessary constraints on the solution. Because cases "A" and "B" did in fact converge to a solution, these results are favored.

The reduction in permeability in the lower horizon post-shot is interesting and suggests that compaction and not permeability enhancement is the predominate mechanism of deformation at shot time in these sediments. Hanson (1984) has shown that, for open-hole analysis and for frequencies typical of barometric pressure records, the averaging radius around the hole is on the order of tens to a few hundreds of meters. Thus, a localized compaction in the vicinity of the shot point could indeed account for these observed results.

Figures 4.32 and 4.33 show the results of multi-layer models applied at U2ff in the frequency domain. The temperature contamination at U2ff was extremely high (see raw data and associated spectra) and no solution was obtainable for Cases "A" and "B". There is no realizable model allowable in which the subsurface pressure at a given frequency can be greater than the surface pressure at the same frequency and the inability of attaining a model convergent to a solution is consistent with this proposition. Results of both cases, with and without frequency weighting, were identical at a statistically significant level, and indicate a permeability decrease with depth.

Figures 4.34 - 4.37 show the multi-layer frequency-domain analysis for chimney U2ev. In all cases, there is an increase in permeability with depth. At a 95% (2-sigma) level, there is considerable overlap between all solutions.

Figures 4.38 - 4.41 show the multi-layer frequency-domain analysis for chimney U19ac. For all cases, the multi-layer analysis indicates a high permeability upper horizon (Timber Mountain Tuff) underlain by a much lower permeability horizon (Paintbrush Tuff) which is in turn underlain by a high permeability horizon (rhyolite lava). These results are consistent with the open-hole pre-shot time-domain analysis (Hanson, 1984), which yielded 44.5 Darcies for the Timber Mountain Tuff, 13.4 Darcies for the Paintbrush Tuff, and 22 Darcies for the rhyolite lava. The latter values assumed all horizons had a connected porosity of 0.01. It is interesting to note that the lower horizon (rhyolite lava), in which the shot occurred, shows an increase of roughly a factor of 2 in permeability between pre-shot and post-shot. One explanation is an increased permeability due to pervasive fracturing in the rhyolite lava due to shock loading at shot time.

It is interesting to note that the multi-layer models in which the tidal constituents were removed suggest a very large permeability for the Timber Mountain Tuff. However, as the figures indicate, this permeability is not constrained - the uncertainty in it is larger than its value. With this in mind, the strongest statement that we can make at this time regarding the permeability of the Timber Mountain Tuff at U19ac is that it is probably greater than 100 Darcies.

In order to determine whether or not we are computing nonsense in the above analyses (which, considering the approximations, assumptions, and nature of the data, is a distinct possibility!), we took the gas flow parameters as determined in the frequency domain analyses and used these to compute forward models in the time domain to compare with the measured downhole data. Figures 4.42 - 4.45 show these results. For all chimneys, with the exception of U2ff, frequency-domain gas flow parameters for Case "A" (tidal constituents retained, no frequency weighting) were used for the forward models. The time-domain data on which all forward models were run had all tidal constituents removed. This was done primarily to "clean up" the data for a better visual comparison of measured and predicted data.

For chimneys U2ev, U2ff, and U2fe, the time-domain prediction showed very good correspondence with the measured in-hole data. Indeed, the fit was better than that expected since the frequency domain analysis was constrained only to match spectral amplitudes - no attempt was made to match phase. As an aside, the reason only amplitudes were matched is due to the fact that the large section of open hole will quite efficiently destroy any phase information in the signal. The time-domain forward model on chimney U19ac showed a significant phase shift with respect to the measured in-hole data (see Fig. 4.45). Visually, the phase shift is associated with the lower frequency components of the signal and seems, to first approximation, to be independent of time. We therefore have attributed the shift to the "initial state" term in equation 3-41, which was discussed in more detail in Chapter III. A more extensive study of this observed phase shift should be carried out before a definitive cause be stated, however.

Figure 4.28. Multi-layer model for U2fe (Case "A"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.29. Multi-layer model for U2fe (Case "B"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.30. Multi-layer model for U2fe (Case "C"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.31. Multi-layer model for U2fe (Case "D"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.32. Multi-layer model for U2ff (Case "C"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.33. Multi-layer model for U2ff (Case "D"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.34. Multi-layer model for U2ev (Case "A"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.35. Multi-layer model for $U2_{ev}$ (Case "B"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.36. Multi-layer model for U2ev (Case "C"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.37. Multi-layer model for U2ev (Case "D"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.38. Multi-layer model for U19ac (Case "A"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.39. Multi-layer model for U19ac (Case "B"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.40. Multi-layer model for U19ac (Case "C"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.41. Multi-layer model for U19ac (Case "D"). Open-hole section indicated by vertical bar. Sensor location chosen at midpoint of open-hole section. Numbers in parentheses are uncertainties (1-sigma).

Figure 4.42. Forward time-domain multi-layer prediction using parameters evaluated from frequency-domain multi-layer inversion - U2fe. (tidal constituents removed)

Figure 4.43. Forward time-domain multi-layer prediction using parameters evaluated from frequency-domain multi-layer inversion - U2ff. (tidal constituents removed)

Figure 4.44. Forward time-domain multi-layer prediction using parameters evaluated from frequency-domain multi-layer inversion - U2ev. (tidal constituents removed)

Figure 4.45. Forward time-domain multi-layer prediction using parameters evaluated from frequency-domain multi-layer inversion - U19ac. (tidal constituents removed)

CHAPTER V

MASS TRANSPORT - BAROMETRIC PUMPING

The past several chapters have dealt with the problem of characterizing the gas flow properties of nuclear chimneys and the surrounding formation. These properties include the hydraulic diffusivity, permeability, and connected porosity as inferred by barometric pressure transient analysis. These parameters taken alone are useful for identifying qualitatively the likelihood that a specific underground nuclear shot site may leak under given in-situ gas pressure conditions. However, until a reasonable time-dependent underground gas pressure distribution is identified and coupled with a convection-diffusion mass transport model, a quantitative description of radioactive nuclide transport to the surface is impossible.

There are two primary mechanisms following an underground nuclear test which can induce gas flow in the formation. The first is obviously the temperature- and compaction-induced overpressure at or near the shot-point which causes flow away from the shot. Estimates of the spatial and temporal pressure distributions assuming both single-phase ideal gas and multiphase flow have been presented in the literature (Olsen, 1967; Morrison, 1973). Due to the impulsive nature of the source, the gas flow induced by the shot diminishes with time. The rate at which the multiphase gas pressure pulse decays, both in space and time, is slower than that of a single phase ideal gas due to effects of condensation and evaporation of resident pore fluid.

The second mechanism that may enhance radionuclide migration from the shot point to the surface is barometric pumping. The frequencies of these pressure signals are sufficiently low to allow for significant pressure variation penetration into the rock at the NTS. Depth of penetration of the pressure signal can be easily approximated by:

$$Z(\text{meters}) = -2.2 \sqrt{k(D) \cdot T(\text{hr}) / \phi] \ln(P/P_s)} \quad (5-1)$$

where k is permeability (in Darcies), T is signal period (in hours), ϕ is formation porosity, P is downhole pressure variation and P_s is surface pressure variation. $\ln$ is the natural logarithm function. Thus, if we wish to know at what depth the surface pressure signal of period 24 hours is diminished by a factor of 1/2 in a formation exhibiting a permeability of 50 Darcies and a porosity of 15%, we have that:

$$Z = -2.2 \sqrt{50 \cdot 24 / 0.15} \ln(0.5)$$

or

$$Z = 136 \text{ meters}$$

Using this simple equation, it can readily be determined that for almost all realistic values of permeability and connected porosity at the NTS, barometric fluctuations at the surface can propagate to depths on the same magnitude as typical underground nuclear shot depths.

Unlike shot-induced gas flow, barometric pressure fluctuations continue indefinitely. The magnitudes of the pressure variation is considerably smaller, however, than shot-induced variations. The former are on the order of 0.1 psi and the latter are several orders of magnitude higher. Depending on the ratio of permeability/porosity, or equivalently, hydraulic diffusivity, barometric pressure fluctuations may account for radioactive gas leaks shortly after (within hours) of an underground nuclear explosion and most certainly will play a major role in long-term radionuclide migration to the surface.

The following discussion addresses the question of enhancement of radionuclide migration due to barometric pumping for conditions similar to those encountered at the NTS. The purpose of this discussion is to develop a simple convection-diffusion model and to use this model to identify the magnitude of the barometric pumping effect. The model will also be used to identify those parameters for which mass transport due to barometric pumping is most sensitive.

5.1 1-D Convection-Diffusion Mass Transport Model

We consider in the following that gas flow and mass transport is limited to the vertical (z) direction. This is equivalent to saying that the radioactive gas created by an underground nuclear test is restricted to an infinite slab at depth Z_s (shot depth) parallel with the earth's surface. It also presupposes that the gas flow properties of the formation from the surface to the shot depth are homogeneous and isotropic and that the surface barometric pressure loading at the surface is uniform. The latter is a very good approximation since the spatial wavelengths of pressure variations is on the order of hundreds of kilometers. We have also assumed single species decay for the radioactive solute. For species whose half-life is short, on the order of hours or at most, a few days, this assumption should be generalized to sequential decay (see for example van Genuchten, 1985).

With these restrictions, the convection-diffusion equation is

given by (Javandel, et al., 1984):

$$D \frac{\partial^2 C}{\partial z^2} - \frac{\partial}{\partial z}(vC) - \lambda C = R \frac{\partial C}{\partial t} \quad (5-2)$$

where:

$C(z,t)$ = solute concentration
 t = time
 z = depth
 $v(z,t)$ = gas velocity
 D = dispersion coefficient
 R = retardation factor
 λ = solute radioactive decay constant
 $\{\ln(2)/\text{half-life}\}$

The gas velocity $v(z,t)$ can be computed independently using either a homogeneous and isotropic half-space or layered half-space geometry with prescribed vertical permeability and porosity distributions and a prescribed surface barometric pressure history. Initial and boundary conditions are required to obtain a unique solution to the convection-diffusion equation. For the case under consideration, these conditions can be represented as:

(1) surface solute flux:

$$-D \frac{\partial C}{\partial z} + vC = KC, \quad z=0 \quad (5-3)$$

(2) source concentration:

$$C(z,t) = C_0 e^{-bt}, \quad \begin{matrix} z=L \\ t>0 \end{matrix} \quad (5-4)$$

(3) initial concentration:

$$C(z,t) = 0, \quad t = 0 \quad (5-5)$$

where:

K = surface mass transfer coefficient
 b = source decay coefficient
 C_0 = initial source concentration

Figure 5.1 shows the geometry of the half-space. Note that the gas velocity is defined for all time and is not limited just to $t > 0$. Prior to $t = 0$, which is here defined as the shot time, the solute concentration is zero. Concentration becomes non-zero only for $t > 0$.

The boundary condition given by eq. (5-5) insures mass balance of the solute flux at the surface. The first term on the left hand side of equation (5-5) is solute flux due to diffusion and the second term to convection. Note that if we set gas velocity v to zero, the surface boundary condition given by equation (5-5) is analogous to that which often occurs in heat transfer at a surface, where for this case, K is the heat transfer coefficient which depends on both material properties and air flow across the surface. One might be tempted to use the somewhat simpler surface boundary condition:

$$C(z,t) = 0, \quad z = 0 \quad (5-6)$$

which assumes that, as soon as the radioactive solute reaches the surface, it immediately dissipates into the atmosphere. This is probably an excellent approximation to reality. However, we point out that equation (5-6) is equivalent to equation (5-5) for the case for K very large (infinite). Indeed, as we shall see, for surface wind speeds a few tens to a few hundreds of meters per hour, we can treat K as infinite. In the following, we will assume the more general boundary condition given by equation (5-5).

If we restrict the gas velocity and dispersion coefficient to

Figure 5.1. Geometry of one-dimensional barometric pumping mass transport model.

be constant in space and time, analytic or semianalytic solutions can be readily found (Javandel, et al, 1984; van Genuchten, M. Th., 1982,1985). However, for the case under consideration, these restrictions are not acceptable. For surface barometric pressure loads, the gas velocity will neither be constant in space nor in time. Furthermore, in general the dispersion coefficient (or, more correctly, the dispersion tensor for flow in greater than one dimension) will depend on velocity (de Josselin de Jong, 1958; Bear, 1961; Bachmat and Bear, 1964). Since the velocity for the case under consideration is not constant, the dispersion coefficient will depend in a complex way on space and time.

We have solved equations (5-2) - (5-5) for the case of velocity and dispersion coefficient constant in space in time. This was done so that we would have a means of checking the validity of the numerical solution in which these restrictions were removed. The semianalytic solution method is outlined in the following and is represented by the Fortran computer program TRANS2 (Transport #2) in the Appendix.

5.2 Semi-analytic Solution of Transport Equations for Constant Velocity and Dispersion Coefficient.

A semi-analytic solution to the above problem can be found in a straight-forward fashion using analytic forward and numerical inverse Laplace transforms. The general form of equation (5-2), subject to condition (5-5), in Laplace transform space is given by:

$$\frac{\partial^2 \hat{C}}{\partial z^2} - \frac{v}{D} \frac{\partial \hat{C}}{\partial z} - \frac{R}{D} (1+1) \hat{C} = 0 \quad (5-7)$$

where s is the transform variable corresponding to time and the "hats" denote transformed functions.

Assuming a solution form of $\exp(\beta z)$, the auxiliary equation (Leighton, 1963) can be found:

$$\beta^2 - \frac{v\beta}{D} - \frac{R}{D}(\lambda+1) = 0 \quad (5-8)$$

The two roots of the quadratic auxiliary equation are:

$$\beta^{\pm} = \frac{\frac{v}{D} \pm \left(\frac{v^2}{D^2} + \frac{4R}{D}(\lambda+1) \right)^{1/2}}{2} \quad (5-9)$$

Thus, the general solution can be written as:

$$\hat{C}(z, \lambda) = A e^{\beta^+ z} + B e^{\beta^- z} \quad (5-10)$$

The two unknown coefficients, A and B, in the above general solution are determined by imposing the surface and source boundary conditions given by equations (5-3) and (5-4), respectively.

The final solution, in Laplace transform space, is easily found to be:

$$\hat{C}(z, \lambda) = \frac{C_0}{(a+b)(\xi_2 - \xi_1)} \left(\xi_2 e^{\beta^+ z} - \xi_1 e^{\beta^- z} \right) \quad (5-11)$$

where:

$$\xi_1 = (v-k)e^{\beta^+ L} - D\beta^+ e^{\beta^+ L}$$

$$\xi_2 = (v-k)e^{\beta^- L} - D\beta^- e^{\beta^- L} \quad (5-12)$$

Note that, as the surface mass transfer coefficient K gets large, the surface solute concentration goes to zero, as pointed out earlier.

Because of the complexity of equation (5-12), a solution in the time domain will be difficult if not impossible to obtain analytically. We therefore have used a numerical Laplace transform inversion algorithm (Stehfest, 1974) to obtain a time domain solution. This algorithm is both fast and accurate. The Fortran computer program TRANS2, given in Appendix I, calculates both spatial concentration distributions for a given time or concentration history at a given location.

5.3 Numerical Solution of Convection-Diffusion Equation

For reasons discussed earlier, neither the gas velocity v nor the dispersion coefficient D (which can depend on v) will be constant in space or time. As a result, equation (5-2) becomes highly nonlinear through the products of $C \cdot v$ and $C \cdot D$, which eliminates the possibility of a straight-forward analytic solution. A numerical solution was constructed using a 5th order Runge Kutta method (Acton, 1970).

Briefly, the Runge-Kutta technique is a single-step time-marching procedure for numerically solving differential equations which are first order in time. As a result, these techniques are ideally suited for parabolic equations, specifically, the diffusion equation. In the present application, we break the region between the shot point and the surface into N layers of equal thickness. These layers are coupled with each other through a Pade' central difference approximation as follows:

$$\frac{\partial C_i}{\partial t} = \frac{D}{R\Delta z^2} (C_{i-1} - 2C_i + C_{i+1}) - \frac{1}{2R\Delta z} (C_{i+1} v_{i+1} - C_{i-1} v_{i-1})$$

$$- \lambda C_i, \quad i=2,3,\dots,N-1 \quad (5-13)$$

where $i=1$ and $i=N$ correspond to the source and surface locations, respectively and where R is the layer thickness. Note that $i=1$ corresponds with the source position ($z = 0$) and $i=N$ corresponds with the surface position ($z = L$). We have chosen this coordinate representation, namely z increasing toward the surface, since the solute concentration decreases toward the surface. The surface mass transport boundary condition, given by equation (5-5), is:

$$C_N(t) = \frac{DC_{N-2} - 4DC_{N-1}}{2\Delta z(v_N - K) - 3D} \quad (5-14)$$

and the source concentration boundary condition is represented by:

$$C_1(t) = v_1 C_0 e^{-bt} + \frac{D[4C_2(t) - C_3(t)]}{3D + 2v_1 \Delta z} \quad (5-15)$$

We therefore can represent the spatially discretized system as:

$$\frac{\partial C_i}{\partial t} = \beta_{i-1} C_{i-1} + \beta_i C_i + \beta_{i+1} C_{i+1},$$

$$i = 2, 3, 4, \dots, N-2$$

(5-16)

$$\frac{\partial C_{N-1}}{\partial t} = (\beta_{N-2} + \beta_N \gamma_{N-2}) C_{N-2} + (\beta_{N-1} + \beta_N \gamma_{N-1}) C_{N-1}$$

where the coefficients β and γ are represented by:

$$\beta_{i-1} = \left(\frac{D}{R\Delta z^2} + \frac{v_{i-1}}{2L\Delta z} \right), \quad \gamma_{N-2} = \frac{D}{2\Delta z(v_N - K) - 3D}$$

$$\beta_i = -\left(\frac{2D}{R\Delta z^2} + \lambda \right), \quad \gamma_{N-1} = \frac{-4D}{2\Delta z(v_N - K) - 3D} \quad (5-17)$$

$$\beta_{i+1} = \left(\frac{D}{R\Delta z^2} - \frac{v_{i+1}}{2L\Delta z} \right)$$

Note that $C(1)$ is computed independently through eq. (5-15). In matrix-vector form, the above system of coupled differential equations can be represented as:

$$\frac{\partial \vec{C}}{\partial t} = A \vec{C} \quad (5-18)$$

where C is the column vector $[C(2), C(3), \dots, C(n-1)]$ and A is an $N-2 \times N-2$ matrix of coefficients made up of the coefficients β and γ .

The 5th order Runge-Kutta marching scheme is given by:

$$y_{k+1} = y_k + \frac{1}{6} (g_0 + 2g_1 + 2g_2 + g_3)$$

where:

$$\begin{aligned} g_0 &= \Delta t f(t_k, y_k) \\ g_1 &= \Delta t f(t_k + \Delta t/2, y_k + g_0/2) \\ g_2 &= \Delta t f(t_k + \Delta t/2, y_k + g_1/2) \\ g_3 &= \Delta t f(t_k + \Delta t, y_k + g_2) \end{aligned} \quad (5-19)$$

In the case under consideration, the solute concentration C represents the function y in equation (5-19) and the matrix operation $[A]C$ represents the function $f(t, y)$ in the Runge Kutta marching scheme. k is the index corresponding to the time step. Using this method, it is very easy to introduce nonlinear behavior and/or time and space dependence of the independent variables. As will be seen, this approach allows for easy modification of the functional form of the dispersion coefficient. This is valuable from the standpoint that there is currently considerable question on just what form the dispersion coefficient should take. The latter is discussed in some detail in a later section.

The numerical Runge Kutta method discussed above has been cast in terms of a Fortran computer program TRANS1 given in the Appendix. We point out here that, although the gas velocity field $v(z, t)$ is computed on the assumption of a homogeneous and isotropic half-space, a modification to the subroutine VEL in TRANS1 to represent a more complex situation (eg. a layered half-space) is easily carried out. We have also restricted the surface barometric pressure to be a pure sinusoid of the form $\exp(i\omega t)$ in order to address the question of frequency sensitivity of mass transport. Again, with straight-forward modification to

subroutine VEL, this restriction can be removed. In particular, if one wished to look at gas transport under an actual surface barometric pressure record, VEL could be modified to compute the impulse response of a surface delta function load, followed by a convolution of the impulse response with the actual surface pressure record.

In order to understand the units, consider the following. If the radioactive gas concentration C_0 is in kilograms per cubic meter, then the surface flux is in kilograms of radioactive gas per square meter per hour. If a different set of units for concentration is used, then the units used for surface flux must be altered accordingly. For example, if the source concentration were taken to be Curies per cubic meter per hour, then the surface flux would be Curies per square meter per hour.

Table 5.1 shows the values of the model parameters used in all of the barometric pumping model runs.

TABLE 5.1

Parameter Values Used In
Numerical Transport Calculations

N (number of layers)	= 21
(time step)	= 0.01 hr.
P_{avg} (mean static gas pressure)	= 85 kPa
R (retardation factor)	= 1
λ (solute decay constant)	= 0
C_0 (initial source concentration)	= 1
b (source decay constant)	= 0

For our initial runs, we assumed a likely "worst case" scenario which may be typical for the fractured volcanics in the mesa areas of the NTS. Hanson (1984) has shown that the hydraulic diffusivity may be as high as $100,000 \text{ m}^2/\text{hr.}$, which reflects permeabilities of roughly 50-60 darcies and porosities of roughly 0.1%. Table 5.2 shows the values of the model parameters used in this calculation.

Fig. 29. Distribution of dispersivities of porous and fractured media [modified from *Lallemand-Barres and Peaudecerf, 1978*].

Figure 5.2. Distribution of dispersivities of porous and fractured media (from Javandel, et al., 1984).

TABLE 5.2

Mass Transfer and Formation Hydraulic
Parameters Used in Numerical Transport Calculations

K (surface transfer coeff.)	= 10 n/hr
D1 (Fickian diffusivity)	= 10 m**2/hr
D2 (dispersivity coeff.)	= 10 m
Df (formation hydraulic diffusivity)	= 100,000 m**2/hr
Zs (shot depth)	= 100 m

The value of D2, the dispersivity coefficient, was chosen based on dispersivities measured in porous and fractured media. A value of 10 m. is conservative for fractured media (see Fig. 5.2).

The first run assumed that a surface sinusoidal pressure history, with a peak amplitude of 1000 Pa and 24 hour period (corresponding to the diurnal atmospheric tide) was driving the transport system (see Fig. 5.3). Figure 5.4 shows the surface solute flux history for the first 100 hours after a shot located at a depth of 100 m. Superimposed on Figure 5.4 is the predicted surface solute flux had there been no surface pressure variations. The latter reflects purely Fickian diffusivity.

It is quite evident that introducing the effect of barometric pumping significantly enhances the surface solute flux. The extra peak observed in each of the flux maxima is due to the fact that, at these times, the surface gas velocity is a maximum. Because the dispersivity depends on gas velocity, the dispersivity increases, thus increasing the flux.

Figure 5.5 shows a break-down of the diffusive and convective terms of the solute flux. The total surface flux shown in Fig. 5.4 is a sum of these two components. Note that the diffusive component is always positive, as required by the nature of any diffusion process. The convective component, however, changes sign, reflecting the direction (up or down) of the gas flow.

Figure 5.6 shows exactly the same situation as discussed above with the exception that the surface barometric pressure has a 12 hour period. It is seen that the basic character of the time history of the surface solute flux is unchanged. At least for this particular case, the amplitude of the surface solute flux is not particularly sensitive to the frequency of the surface barometric pressure record. Figure 5.7 shows the break-down of the diffusive and convective terms of the solute flux.

The velocity dependence of the dispersion coefficient was "switched off" by setting $D2 = 0$, all other parameters kept

fixed. Figures 5.8 and 5.9 show the result of this alteration for surface barometric pressure signals of 24 hour and 12 hour periods, respectively. As one might expect, the computed surface solute flux for the cases in which the surface barometric pressure is either "on" or "off" track each other in time. This identifies clearly the fact that the enhancement of solute transport by barometric pumping is through the velocity dependence of the dispersion coefficient.

In the next set of numerical experiments, the shot depth was increased to 300 meters, all other parameters remaining the same. The surface pressure fluctuation was assumed to have a 1000 Pa amplitude and 24 hour period. Figure 5.10 shows the surface solute flux history for this situation. It was found that the flux amplitude with the surface barometric pressure switched off was 3 orders of magnitude smaller than with the pressure switched on, again underscoring the significance of this transport mechanism. The increased shot point depth delayed the first arrival of the surface flux due to the increased diffusion time to travel this distance. The amplitude of the surface flux was also decreased by 5 orders of magnitude.

5.4 Discussion

The role of barometric pumping in enhancing the migration of radioactive gas from the shot point to the surface has been demonstrated to be a significant transport mechanism. The largest uncertainty in the above modelling effort is the functional form of the dispersion coefficient. For porous sediments, the linear dependence of dispersivity on gas velocity is probably a good approximation (Bachmat and Bear, 1964). Probably the largest uncertainty for porous sediments is the value of D_2 . Most work carried out historically in dispersive systems similar to the one under consideration have been for saturated sediments. Dispersivity calculated from column tests on relatively uniform porous media ranges between 0.01 cm. and 1 cm.. Another way of determining dispersivity is by using either single-well or double-well tracer tests. Values of dispersivity obtained by these methods are generally several orders of magnitude larger than the range obtained in the laboratory tests. Figure 5.2 shows typical dispersivities of porous and fractured media (Javandel, et al., 1984). Note that observed dispersivity in fractured media can get as large as several hundreds of meters, an order of magnitude greater than the 10 meters used in the above examples.

A second uncertainty is in the value of K , the surface mass transfer coefficient. As we have pointed out earlier, however, in general this coefficient can be set to infinity with little effect on the result. Figure 5.11 shows the computed surface solute flux history for $K = 10$ m/hr, 100 m/hr, and 1000 m/hr for a 24 hour period surface pressure variation and for the previous

values of formation parameters. Note that, although there is some difference in surface flux between the cases for $K=10$ m/hr and 100 m/hr, above $K=100$ m/hr, there is no significant change.

There is both theoretical and experimental evidence that dispersivity in fractured formations may not be proportional to gas velocity but may instead be proportional to distance traveled (Neretnieks, 1981). Different fissures may have different flow velocities, and the set of individual pathways from the shot point to the surface may also have considerable variations in travel times. Without further analysis, one cannot immediately say just what kind of effect this different functional dependency for dispersivity may have on the reported analysis. One might expect, however, that cumulative solute transfer to the surface from the shot point might be larger for long times since distance is monotonically increasing whereas gas velocity is bounded for a given surface pressure signal frequency.

The value of molecular (Fickian) gas diffusivity used in the above analysis was chosen rather arbitrarily prior to carrying out a literature search. Subsequently, we have determined that the value used (namely $10 \text{ m}^2/\text{hr}$) is one to two orders of magnitude high for gas diffusion through a porous medium. Table 5.3 documents result of past investigations on this parameter (Evans, 1959). However, as we have pointed out, the contribution of molecular diffusion to the net solute transport is small when compared with the dispersive component. Therefore, the results presented, at least for the 300 m depth of burial, is relatively unaffected by this error.

Figure 5.3. Surface atmospheric pressure variation used for diurnal (24 hour period) transport models.

Figure 5.4 Surface solute flux with barometric pumping (solid) and without barometric pumping (dashed) - 24 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.5. Diffusive (solid) and convective (dashed) components of surface flux with barometric pumping - 24 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.6. Surface solute flux with barometric pumping (solid) and without barometric pumping (dashed) - 12 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.7 Diffusive (solid) and convective (dashed) components of surface flux with barometric pumping - 12 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.8. Surface solute flux assuming dispersivity independent of gas velocity, With barometric pumping (solid) and without barometric pumping (dashed) - 24 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.9. Surface absolute flux assuming dispersivity independent of gas velocity, with barometric pumping (solid) and without barometric pumping (dashed) - 12 hour period surface pressure variation. (shot depth = 100 m.)

Figure 5.10. Surface solute flux with barometric pumping (solid) and without barometric pumping (dashed) - 24 hour period surface pressure variation. (shot depth = 300 m.). (Note: dashed curve is effectively superimposed on x-axis).

Figure 5.11. Comparison of surface solute flux for $K = 10$, 100 , and 1000 m/hr. Minimum amplitude curve (solid) corresponds to $K=10$ m/hr. Maximum amplitude curve (dashed) corresponds to $K = 100, 1000$ m/hr which are effectively superimposed.

TABLE 5.3

Diffusion Coefficients of Radioactive Gases
in Various Media

(from Evans, 1959)

Source	Radioactive gas	Medium of diffusion	Measured diffusion coefficient cm^2/sec
Baranov and Novitskaya 1949	radon	quartz sand, dry	6.75×10^{-2}
	thoron	quartz sand, dry	6.75×10^{-2}
	thoron	quartz sand, 10.4% moisture	3.75×10^{-2}
	thoron	quartz sand, 15.2% moisture	1.00×10^{-2}
	thoron	powdered clay, air dry	5.00×10^{-2}
	radon	water, 18° C	$1.15 \times 10^{-5} *$
	radon	air	0.1 *
Aliverti and Lovera 1949	radon	air	0.1 *
		soil	0.013
Hirst and Harrison 1938 and 1939	radon	argon at 760mm and 15° C	0.092 *
		air at 760mm and 15° C	0.120 *
Israel and Becker 1935	radon	soil air	0.05
Mortari, 1933	radon	air	0.11 *
Eckmann, 1913	radon	air	0.07 *
Chaumont, 1910	radon	air	0.1014 *
	radon	air	0.1017 *

* True diffusion coefficients.

TABLE 5.3 (Cont'd)

Source	Radioactive gas	Medium of diffusion	Measured diffusion coef- ficient cm ² /sec
Leslie, 1912	thoron	air	0,085 *
	actinon	air	0,098 *
Bagnall, 1957	radon	water	$7,6 \times 10^{-5}$ *

* True diffusion coefficients.

CHAPTER VI

DISCUSSION AND CONCLUSIONS

The data and analyses presented in this report serve well to point out a number of different aspects of barometric pressure transient testing at the Nevada Test Site. The technique is ideally suited for evaluating gas flow parameters at the NTS at depths on the order of nuclear shot depths due to the fact that the nature of the subsurface formations in this area allow for deep penetration of surface atmospheric pressure variations. However, the results of this study indicate that long term containment of radioactive gas generated at shot time may be compromised as a result of these formation properties. In the following, we will discuss the results presented in this report in terms of data acquisition procedures, interpretation in terms of modelling, how best the techniques discussed can be improved for future testing, and impact on the overall goals of the LLNL Containment Program. Because of the broad scope of information presented in this report, we have broken the discussion into several sections, each of which addresses what we feel are key issues.

6.1 Chimney Models and Data Acquisition - General Comments on Methodology and Procedure

Work carried out historically at five nuclear chimneys was determined to be basically correct in that published results of this historic work were duplicated in the present study. The interpretation models used historically to evaluate the gas flow properties within and immediately surrounding the chimneys was the simplest available - namely, the homogeneous and isotropic half-space. This model assumes that both chimney and formation properties are identical and are spatially homogeneous and isotropic. As a result, the model does not allow the capability of calculating differences in gas flow properties between chimney and formation - a result which would be very useful to know. Little is known at present on just how the initial shock loading at shot time and the subsequent chimney collapse will affect the gas flow properties in the resulting chimney.

The current work on recently acquired chimney data suggests that the choice of models will greatly influence interpretation. For example, a homogeneous and isotropic half-space model applied to barometric pressure data at U19ac post-shot indicated a diffusivity of $28580 \text{ m}^2/\text{hr}$. (Table 4.8), which translates to 19 Darcies under the assumption of a 0.01 connected porosity. However, a multi-layer model applied to the same data indicates that, depending upon which formation horizon one is considering, the permeability could range anywhere from roughly 9 Darcies to

something greater than 100 Darcies (see Figs. 4.38 - 4.41), again assuming a 0.01 connected porosity. As it turns out, the shot-point at U19ac was placed beneath the "tightest" formation, which will improve containment. However, if one had available only those results pertaining to the half-space model, he may have taken a somewhat more pessimistic outlook on containment.

The applicability of the model used in data interpretation depends not only on the a priori perception of the geometry of the structural system one is trying to understand (in this report, the chimney-formation system) but also depends critically upon how the data is taken. Specifically, we are talking about the spatial extent of the observation port - in the current case, the section of hole beneath the casing in the slant hole open to the formation. A long open-hole section will perturb the gas flow geometry about the measurement port much more than a very short open-hole section, as was shown by Hanson (1984). Unless the model can account for this perturbation in some way, there can again be errors made in interpreting the results of the modelling effort. Historical efforts addressing chimney permeability took the appropriate precautions and, through grouting and perforating, isolated the subsurface measurement port to an effective "point-response" port. However, more recent efforts at U2fe, U2ev, U2ff, and U19ac simply left the section of hole beneath the casing open. This section of hole was typically a large fraction of the total hole depth. In both historic and recent efforts, the slant hole was open to the chimney at the chimney-formation boundary.

In principle, this is no problem. Since we think we know the approximate geometry of the chimney-formation system (a supposition that should be verified), the location of the open-hole section of the measurement port, and typically, the lithology (stratigraphy) of the surrounding formation through logs, the problem is well-posed at least in terms of forward models. However, data interpretation is an inverse problem. This opens up problems of very practical nature. The inverse problem of fitting a fully three-dimensional gas flow geometry to data will likely absorb a significant fraction of the annual budget of a medium-sized earth sciences laboratory, or at least tie up its computational facility for unacceptably large blocks of time. Thus, it is to our advantage to reduce the dimensionality of the gas flow geometry as much as possible prior to interpretation so as to reduce this computational effort. We have been told that the section of hole beneath the casing in the slant holes for recently acquired chimney data on U2fe, U2ff, U2ev, and U19ac was left open to minimize cost. We suggest that, in light of the above discussion, a critical look be taken by the LLNL Containment Program at this "cost reduction" scheme.

Forgetting for the moment the problems outlined above regarding the slant hole measurement port, we must point out that in general, the gas flow geometry in a chimney-formation system is, at a minimum, two-dimensional (radial and vertical). This presupposes that the system has cylindrical symmetry about the axis of the chimney. We have found that, although computationally time consuming, inverse problems on two-dimensional systems can be carried out on this kind of pressure transient testing. This is documented by the work by Hanson (1984) on "open-hole" formation analysis. Historically acquired chimney data acquisition forced the measurement port to be spatially limited. On the assumption that the chimney-formation systems at these chimneys is axisymmetric, the data can be interpreted in terms of two-dimensional models - a realizable goal based on our past experience with open-hole analysis. However, the introduction of an extended measurement port, as used in the recently acquired chimney data acquisition, forces the geometry to be three-dimensional. We can safely say that a full three-dimensional interpretation of this data is beyond the scope of almost all practical interpretation efforts.

We suggest that more effort be placed on interpreting the historical chimney data since: (1) the surface and subsurface barometric pressure data now exists as a result of this project and (2), the nature of the slant hole completion in this historic data is such to allow a simpler model to fully characterize the chimney-formation system than the recently acquired chimney data would require.

Unfortunately, we do not at present have sufficient information regarding the stratigraphy at these sites, or even for that matter, where the sites are located. Evidently, this information has been lost in the shuffle, although we know it still exists (personal communication, Dr. Joseph Hearst, LLNL). We recommend that a minimal effort be carried out by someone familiar with the NTS data base to try to recover this information.

6.2 Thermal Contamination

Another question which needs to be addressed is the problem of thermal contamination of the pressure signals. Historical chimney analysis simply ignored this problem - indeed, we have seen no evidence in past publications that thermal contamination was even considered a problem. However, the current project, and some and previous work (Hanson, 1984), has showed that this signal contamination can be a problem. There are several methods by which this problem can be minimized. In this and previous work (Hanson, 1984), a line spectral analysis on the surface and pressure signals has been carried out for the purpose of removing all information at the tidal frequencies. This, however, may also remove some very useful higher frequency data corresponding to the small but present non-solar atmospheric tides. This higher frequency information may be required to constrain more

sophisticated models - for example the multi-layer model at U19ac in this report.

Since the principal thermal contamination will occur at specific solar tidal frequencies, for example the K1, S1, S2, and S3, this procedure should minimize the problem. No attempt has been made to remove just the solar tides, however. The main reason for this was expediency - the current code configuration is an "all or nothing" procedure. However, the solar tides lie very close to non-solar tides in terms of frequency, and separation of this sort is difficult on data record lengths less than many months duration. We suggest that there exist several "cheap" methods of reducing thermal contamination. The most obvious is to insulate the slant-hole casing and tubing to the pressure gauge where they are exposed to direct solar radiation. A back-hoe could, in the space of a few minutes, bury the casing head under several feet of earth. The tubing and attached pressure gauge could be treated identically. The pressure gauge monitoring surface barometric pressure could be housed in a insulated box with an access port to the atmosphere. Finally, if we are dealing with quartz pressure gauges, which typically are supplied with algorithms for temperature compensation (eg. Peroscscientific Model AS-15), a full temperature correction could be easily carried out with the appropriate placement and monitoring of high-precision thermometers (ie. thermistors).

6.3 Model Uniqueness

With all of the uncertainties introduced due to problems associated with data acquisition and data quality discussed above, an obvious question to be asked is whether or not the solution is unique. A non-unique solution is simply one solution in a family of solutions that can all fit the data equally well, given all solutions are based on the same model. The measure of "fit" to the data will be influenced not only by the number of free parameters in the model but by noise contamination in the data. This problem has been recognized previously (Hanson, 1984) for models more sophisticated than the simple single parameter half-space model. Model uniqueness is not debatable for a single-parameter model - for example, the homogeneous and isotropic half-space model which depends only on hydraulic diffusivity. There will be one, and only one, value of diffusivity that yields a "best fit" of model to data. Even if the wrong model is applied, for example a homogeneous and isotropic half-space model to an actual layered half-space situation, this statement holds true. Again, there will be only one value of diffusivity that fits the data - the only difference is that in this case, the solution will be wrong (from the standpoint of representing the actual geometry). In the following discussion, the differentiation between "wrong" solutions and "non-unique" solutions should be kept in mind.

For barometric pressure transient testing, in which the physical process is governed by the diffusion equation, it is prudent to choose a theoretical model with the least number of free parameters but which can be expected to reasonably approximate the actual structural situation. This is due to the fact that solutions to the diffusion equation can be cast in a series of exponentials of the form $\exp(-bt)$, where t is time. The number of exponentials in this series is roughly the number of free parameters in the model. By free parameters, we mean the number of degrees of freedom in the model. For example, a two-layer half-space model can be shown to have 3 degrees of freedom: two values of diffusivity (one for each layer) and the ratio of permeabilities for both layers.

The uniqueness problem was not encountered in the previously published analyses of the historic chimney data. This is due to the fact that these investigators' choice of models, namely the homogeneous and isotropic half-space model, guaranteed uniqueness. This seeming advantage is obtained, of course, at the expense of understanding the spatial dependence of permeability in and about a nuclear chimney. Their results, and our duplication of these results, are "wrong" from the sense that this degree of model sophistication is well below the a priori understanding of the chimney-formation structure.

More recent analyses of barometric pressure transient testing at the Nevada Test Site (Hanson, 1984) considered more sophisticated models in the interpretation of this type of data. In particular, a partially cased but otherwise open hole intersected a layered half-space. This model was felt to be the minimum configuration (i.e. minimum number of free parameters) that could realistically represent the actual geometry. Layer thicknesses were constrained by hole logs. The most controversial analysis using this model was that carried out at U19ac on the Pahute Mesa. This hole intersected volcanics which can support pervasive cooling cracks and is, to our knowledge, the first hole completed entirely in volcanics that has been the target of barometric pressure transient testing. A three layer half-space, corresponding to the Timber Mountain Tuff, Paintbrush Tuff, and rhyolite lava horizons (in increasing depth), was used in the modelling effort. The model was constrained to three free parameters (permeabilities of each layer) by forcing the connected porosities of each layer to be fixed at 0.01. Resulting calculated permeabilities for the Timber Mountain Tuff, Paintbrush Tuff, and Rhyolite lava were found to be 44.3 D, 13.4 D, and 22 D, respectively. These values of permeability were consistent in magnitude with values calculated through groundwater pump tests in the same area (Blankenagel and Weir, 1973).

The controversy of these results stemmed in large part from the large hydraulic diffusivities inferred from the above results, which could be as high as 100,000 m^2/hr . This value was thought to be unacceptably large by those critiquing the

report, although no substantiation of the "unreasonableness" of this value, other than their personal experience with sediment-derived porous media, was offered. Indeed, if one used a typical value of sediment porosity (say 20%) in this analysis, the permeability of the Timber Mountain Tuff would have been calculated to be 670 D, as reported in Hanson (1984). This value is indeed high for reported conventional pump test permeabilities in fractured hard rock. Work by Snow (1968) and others, substantiate the proposition that connected porosities in fractured hard rock, including volcanics, are typically 1% or less.

Since this investigation allowed for multiple layers, the question again arose regarding model uniqueness (Hanson, 1984). Were there other values of permeability that could be assigned to each of the horizons at U19ac which would fit the data equally well? In particular, a much larger section of hole was open to the formation (19 m - 700 m) in this earlier test at U19ac than in the more recent tests reported here, making the inverse problem even more ill-posed. Due to the large amount of computer time used in these 2-D inverse problems, this question was not answered. However, we point out here that conventional reservoir testing routinely carries out inverse solution models that contain several free parameters. Indeed, we have been responsible for successfully carrying out some of the earliest applications of pressure transient inversion work on deep fractured tight oil wells and on tight gas sands (Hanson, 1984b). As a result, we did not find the question of model uniqueness on so limited a number of free parameters as pressing as others less familiar with the with state-of-the-art in situ testing procedures.

Although not offered as proof of model uniqueness, it is significant that the results reported here for U19ac using a three-layer model (Timber Mountain Tuff, Paintbrush Tuff, and rhyolite lava) are consistent with results obtained previously. The principal difference is a larger inferred permeability post-shot near the shot depth, a difference which is easily explained by shock-induced fracturing. These results were carried out in the frequency domain which allowed control over the higher frequencies, forcing them to have more influence on the inverse solution. Results reported by Hanson (1984) permeability structure at U19ac, and this report for U19ac are similar, in spite of the fact that (1) casing depths are very different (19 m. in the earlier work and 387 m. in this report) and (2) earlier calculations were carried out in the time domain whereas the current result were computed in the frequency domain. This agreement suggests a commonality which can only be attributed to the hypothesis that the vertical permeability distribution computed in both the earlier open hole analyses (Hanson, 1984) and the present work represent the true vertical permeability at U19ac. We also point out that the result reported here for a 2-layer model for U2fe are consistent with previously investigations (Hanson, 1984).

These conclusions are further substantiated with borehole camera surveys at U19ac. From the surface to a depth of roughly 400 m, cooling crack density range from "minor" to "strong". At depths between 400 m. and 600 m., no cooling cracks are evident (personal communication, J. Wagoner, LLNL). These observations are qualitatively consistent with our interpretation that a near-surface horizon (Timber Mountain Tuff) is underlain by a much "tighter" horizon (Paintbrush Tuff). Unfortunately, the camera log information made available to us does not go deeper than 600 m.

The above observations suggest that results reported to date on models of greater sophistication than the simple half-space model can be considered "close to the mark" in terms of uniqueness. However, the maximum number of free parameters in a structural model (i.e. model complexity) that can be dealt with using this technique has yet to be quantified. This difficult question will be resolved only after a much more quantitative investigation is carried out. An ideal candidate for this investigation is the recently acquired data on steamed emplacement holes at the NTS. Multiple sensors are deployed at several depths within these holes which will allow for a highly constrained multi-layer solution. Having established, from all sensor data, the vertical distribution of permeability, the inverse problem can then be carried out on a limited number subsurface sensors to establish at what point there is insufficient data to appropriately reflect the true vertical permeability distribution.

6.4 Assumptions Made in Multi-Layer Models

After the preamble made in section 6.1 regarding dimensionality of models and the necessity of retaining sufficient complexity within the model to reflect the (assumed) chimney-formation structure, the question will certainly arise as to why a multi-layer half-space model was chosen rather than the more sophisticated numerical finite difference model presented in this report. The reason was of practical nature - our computer capability (an IBM-PC, with lots of bells and whistles, but no speed) is limited, and an inverse solution for a 2-D numerical model is beyond out of question. We recommend that those at LLNL involved in this project use the finite difference inverse model (TDCA#1-TDCA#2) listed in Appendix I to reanalyze the recently acquired chimney data at U2fe, U2ff, U2ev, and U19ac.

The layered half-space model was chosen over the semi-analytic cylindrical chimney model for following reasons: (1) as has been reported historically, there doesn't seem to be a large difference in gas flow properties between a chimney and the adjacent formation (see Table 1.1). However, from conventional groundwater pump test analyses (Blankennagel and Wier, 1973), air injection tests (Snoeberger, et al., 1971), and multi-layer barometric pressure transient analyses (Hanson, 1984), there can

be much more significant changes in permeability with depth. The cylindrical chimney model discussed in this report does not allow for a vertical change in permeability. Because of this, we favored the multi-layer half-space model for the current project.

6.5 Enhancement of Radionuclide Migration by Atmospheric Pumping

The results presented in Chapter V regarding the influence of barometric pumping on transport of radioactive gas near the shot point to the surface gives one significant pause for thought. These results suggest that long-term (but possibly low level) leakage due to "breathing" will be the rule rather than the exception in all areas of the NTS where the shot is not below a very good flow containment barrier. In the alluvium regions of the NTS, such barriers to flow may be certain horizons of volcanic nature underlying the sediments. However, the lowest in situ permeability reported for these horizons is 1 or 2 Darcies (Snoeberger, et al., 1971). These permeabilities will impede but not eliminate transport.

The situation is somewhat worse for the Mesa regions of the NTS. Gas flow in these areas will be dominated by fracture porosity (Blankennagel and Wiar, 1972). Most of these fractured formations exhibit very high hydraulic diffusivities due to the very small connected porosities of the bulk fractured material. The gas velocity within the fractures due to surface atmospheric pressure variations is proportional (roughly) to the square root of diffusivity, ignoring for the moment the overpressure at the shot point at shot time which will tend to drive gas and/or fractures toward the surface. The sensitivity of gas velocity to porosity can be better seen by recognizing that, for a given gas flux, a smaller-aperture fracture will require a greater gas velocity. The small aperture fracture translates, however, into a small connected porosity or a large hydraulic diffusivity. Thus, not only does the high diffusivity for these regions allow a very great depth penetration of surface pressure variations, the induced gas velocity (which is chiefly responsible for getting the gas to the surface through a velocity-dependent dispersion) is also enhanced.

The Containment Program's principal concern is avoiding catastrophic leaks shortly after (hours to a few days) after shot time (personal communication, B. Hudson, LLNL). The results of the simulations reported here suggest that the initial emergence of the solute (radioactive gas) at the surface following a shot is very sensitive to shot depth. In the "worst-case" scenario for fractured volcanics discussed in Chapter V, initial emergence will occur within minutes to hours after the shot for a shot depth of 100 m. We recognize that this is a most unrealistic shot depth - we simply use it for comparison and illustration. Under the same situation, but for a shot depth of 300 m., emergence time was increased to roughly 3 days.

The calculated depth sensitivity of solute emergence time suggests that, if a steam-driven crack(s) can be driven to within 200 to 400 meters of the surface for a shot at depth 500 or 600 m., the length of time it would take the solute to reach the surface would be decreased by orders of magnitude. Furthermore, if the crack is propped open, either by material broken loose by the blast or by a shear displacement along the plane of the crack, a significant amount gas may be transported to the near surface horizon due to both free and forced convection within the crack. If the near-surface horizon exhibits a large permeability (eg. Timber Mountain Tuff on Pahute Mesa, NTS), atmospheric pumping may be quite effective on transporting the radioactive gas the remaining distance to the surface.

Clearly more sensitivity runs need to be carried out with the transport model (see TRANS1, Appendix I) before this discussion can be more thoroughly quantified. We have considered only a "worst case" scenario in this report. However, this "worst case" scenario presented in this report has considerable significance in the fact that the gas flow parameters used in it have been measured and reported (this report, for example) in the Mesa regions of the NTS.

6.6 Improvement of Pressure Transient Testing Techniques

Finally, one must pose the question as to how the barometric pressure transient technique might be improved for future testing efforts at the NTS. There are several immediate things one can do - some inexpensive, some not. The good news will be discussed first.

6.6.1 "Cheap" Improvements

The word "cheap" is used somewhat loosely in that, in practice, it must be defined in terms of the worth to the purchaser of the object (or service, or result, ...) being purchased. In the following, we describe what we feel are easy and inexpensive improvements to barometric pressure transient testing data acquisition and analysis, based on what we consider should be the worth to the LLNL Containment Program of the information resulting from this kind of analysis. The cost of these suggested improvements should also be weighed in terms of the only alternative testing technique shown to work at the NTS: mobilizing the equipment necessary for conventional air injection test and carrying out these tests.

Should some feel that these procedures are really not necessary or can be put off some indeterminate time, we suggest that they remove their data acquisition hats for a while and put on their modelling and interpretation hats. We suspect that a few attempts at interpreting less than optimal data will have a significant effect on this viewpoint!

(1) Thermal Contamination

The first problem that can easily be overcome, described earlier, is that of thermal contamination of the data. Some methods by which thermal contamination can be removed from the data can be achieved have been presented earlier - there are probably others. The methods are straight-forward and require no further discussion.

(2) Isolation of Subsurface Measurement Port

Where a partially cased drill hole is used to access the subsurface pressure, it is recommended that the spatial extent of the section of hole exposed to the formation be limited. This can be carried out using a packer-tubing assembly backed by stemming (grout) to the casing or actually to deploy the pressure gauge at the bottom of the hole, again backed by stemming. A third alternative is simply to case the hole the total length and perforate at the bottom. These geometries are shown in the following figures.

For chimney analysis, in which the slant hole is always drilled to one side of the chimney and not along the chimney axis, these procedures will guarantee a reduction of the problem from 3-D gas flow to 2-D (radial and vertical) gas flow, and hence greatly simplify the analysis. For formation analysis where the formation is undisturbed by, for example, a nuclear shot, the geometry can probably be considered a layered half-space. For this case, the reduction in gas flow geometry dimensionality is from 2-D (radial and vertical) to 1-D (vertical) following this procedure.

6.6.2 "Not So Cheap" Improvements

(1) Multiple In-Hole Sensors

The first modification to the testing procedure that falls in this category is to deploy multiple downhole pressure sensors, each of which is spatially isolated in terms of pressure communication with the formation. Multiple subsurface measurement ports will have a much better likelihood of yielding a unique solution for complex structural models than a single measurement port.

An effort is currently under way within the LLNL Containment Program to deploy multiple gauges in stemmed emplacement holes for the purpose of barometric pressure transient testing. The structural geometry for this situation will be either 1-D (layered half-space) or 2-D (several open-hole sections in a layered half-space), depending upon the permeability and depth of the stemming materials used. We expect that multiple subsurface

Figure 6.1. Packer-tubing-stemming completion of slant hole.

Figure 6.2. Packer-gauge-stemming completion of slant hole.

Figure 6.3. Perforated casing completion of slant hole.

sensors will greatly improve resolution in the subsurface vertical permeability distribution. These results, if successful (and we have every reason to believe they will be) should serve as a guide for future barometric pressure transient data acquisition.

(2) A Second Nearby Slim Hole for Chimney Analysis

For the case of chimney-formation gas flow analysis, a significant improvement would be to drill and instrument with multiple subsurface pressure sensors a second hole some distance (say 0.25 to 0.5 km) from the chimney. In this manner, the formation permeability distribution could be calculated independently, and would effectively improve the chances of detecting a vertical change in permeability in the chimney.

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APPENDIX I

Computer Program Listings

Comment:

All programs were written to run on an IBM-PC
(or compatible) system running under MS-DOS.
Programs are written in MS Fortran V3.2

TRANSPORT CODES

- (A) TRANS1: 1-D RUNGE-KUTTA SOLUTION FOR GAS TRANSPORT FROM THE SHOT POINT TO THE SURFACE. ARBITRARY GAS VELOCITY.
- (B) TRANS2: 1-D SEMI-ANALYTIC SOLUTION (CONSTANT GAS VELOCITY)

```

C *****
C +//////////////////////////////////////////////////////////////////+
C +///////////////// TRANSl (Transport #1) ///////////////////+
C +//////////////////////////////////////////////////////////////////+
C *****
$DEBUG
$NOFLOATCALLS
$LARGE
PROGRAM TRANSl

C
C TRANSPORT IS A 1-D CONVECTION-DIFFUSION MODEL THAT SOLVES
C THE EQUATION:
C
C 
$$D*[d^2C/dx^2] - [d(CV)/dx] - LAMBDA*R*C = R*[dC/dt]$$

C
C SUBJECT TO THE BOUNDARY CONDITIONS:
C
C (A)  $-D*[dC/dx] + VC = KC, \quad X=XL$ 
C
C (B)  $C = C0 \exp(-ALPHA*T), \quad X=0$ 
C
C PARAMETERS:
C C(X,T) SOLUTE CONCENTRATION
C D(V) SOLUTE DIFFUSIVITY (=D1 + D2*ABS(V))
C LAMBDA SOLUTE DECAY RATE
C R RETARDATION FACTOR
C V(X,T) SOLVENT VELOCITY (SUPPLIED BY FUNCTION VEL)
C K SURFACE CONVECTION COEFFICIENT
C C(0,T) SOLUTE SOURCE TERM (SUPPLIED BY FUNCTION FUN)
C
C METHOD OF SOLUTION:
C 5th ORDER RUNGE KUTTA SOLUTION IN TIME. THE DOMAIN  $0 \leq X \leq XL$ 
C IS BROKEN DOWN INTO N-1 LAYERS OF UNIFORM THICKNESS. EACH OF THE
C LAYERS IS COUPLED WITH THE ADJACENT LAYERS THROUGH A FIRST ORDER
C (IN TIME) DIFFERENTIAL EQUATION CONSTRUCTED FROM THE PADE'
C CENTRAL DIFFERENCE EXPANSION (IN SPACE) OF THE CONVECTION-
C DIFFUSION EQUATION. NOTE: SOLUTION IS SUBJECT TO INSTABILITY
C DEPENDING UPON CHOICE OF DT AND DX (A TYPICAL PROBLEM WITH THE
C RUNGE KUTTA METHOD). IF INSTABILITY OCCURS, REDUCE DT.
C
C WRITTEN BY: JONATHAN M. HANSON
C HANSON & ASSOCIATES
C SALT LAKE CITY, UT
C JULY, 1985
C
C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON/ROCK/PAVG,DIFF,OMEGA,AMP,MFLAG,V
COMMON/SOURCE/C0,ALPHA
COMMON/PRESS/PRES
DIMENSION G(5,500),C(500)
DIMENSION XX(4,2000),YY(4,2000),ILINE(2),JLINE(2),NPTS(2)
CHARACTER*20 FNAME,GNAME,HNAME
REAL*4 XX,YY,B1,B2,B3
INTEGER*4 ILINE,JLINE

```

```

C
C   TRANSPORT MODEL PARAMETERS
C   XK   ...   SURFACE SOLUTE TRANSPORT COEFF. (M/HR)
C   XLAM ...   SOLUTE DECAY COEFFICIENT (1/HR)
C   R    ...   RETARDATION FACTOR
C   D1   ...   SOLUTE MOLECULAR DIFFUSION COEFF. (M**2/HR) (FICK'S LAW
C
C   D2   ...   MIXING COEFFICIENT (M).
C   XL   ...   DEPTH OF SOURCE
C   NOTE ...   NET DIFFUSION COEFFICIENT IS GIVEN BY:
C               D = D1 + D2*ABS[V(X,T)], WHERE V IS GAS VELOCITY
C
C   SOURCE MODEL PARAMETERS
C   C0   ...   INITIAL SOURCE CONCENTRATION
C   ALPHA...   DECAY CONSTANT FOR SOURCE
C
C   GAS VELOCITY FLOW PARAMETERS INCLUDE:
C   DIFF ...   FORMATION DIFFUSIVITY (M**2/HR)
C   PAVG ...   AVERAGE FORMATION GAS PRESSURE (PA)
C
C   CONTROL PARAMETERS
C   NXOUT...   SPATIAL CONCENTRATION PROFILE PLOTTED EVERY NXOUT
C               TIME STEPS
C   NTOUT...   SURFACE DIFFUSIVE, CONVECTIVE, AND TOTAL SURFACE
C               SOLUTE FLUX WRITTEN TO FILE EVERY NTOUT TIME STEPS
C   MFLAG...   =1, VELOCITY IS PRESCRIBED AND IS INDEPENDENT OF
C               SPACE AND TIME
C               =0, VELOCITY IS COMPUTED USING FUNCTION VEL
C   DT    ...   TIME INCREMENT IN MARCH
C   N     ...   NUMBER OF LAYERS
C
C   SURFACE PRESSURE PARAMETERS INCLUDE:
C   AMP   ...   SURFACE PRESSURE AMPLITUDE (PA)
C   OMEGA...   ANGULAR FREQUENCY OF SURFACE PRESSURE SIGNAL
C   NOTE...   MODEL ASSUMES A HOMOGENEOUS AND ISOTROPIC
C               HALF-SPACE AND A SURFACE PRESSURE SIGNAL OF THE
C               FORM  $P(X=0)=AMP*EXP(I*OMEGA*T)$ 
C
C   REQUIRED FUNCTIONS:
C   VEL(X,T) ... CALCULATES GAS VELOCITY AT DEPTH X AND TIME T
C   FUN(T)    ... CALCULATES THE SOURCE CONCENTRATION. HAS THE
C               FORM  $C(XL,T)=A*EXP(-ALPHA*T)$ 
C
C   ILINE(1)=1
C   JLINE(1)=7
C
C   PI=3.1415926500
C
C   ----- MODEL AND CONTROL DATA INPUT -----
C   READ INPUT DATA FILES
C   WRITE(ID2,5000)
C   READ DATA FROM A DISK DATA FILE
C   READ(ID1,5010) FNAME
C   OPEN (20,FILE=FNAME, STATUS='OLD')
C   READ(20,*) N,XL,DT,TMAX,NXOUT,NTOUT
C   READ(20,*) PAVG,DIFF,F,AMP,MFLAG,V

```



```

C      READ(20,*) XK,XLAM,R,D1,D2,C0,ALPHA
C      -----
C      WRITE(ID2,5020)
C      READ(ID1,5010) GNAME
C      OPEN(21,FILE=GNAME, STATUS='NEW')
C
C      IF(MFLAG.EQ.1) GOTO 20
C      WRITE(ID2,5030)
C      READ(ID1,5010) HNAME
C      OPEN(22,FILE=HNAME, STATUS='NEW')
C
C      UNITS OF INPUT DATA FROM DISK FILE:
C      XL ... M
C      DT ... HR
C      TMAX...HR
C
C      FORMATION GAS VELOCITY MODEL
C      DIFF ..M**2/HR
C      PAVG ..PA
C      F ... 1/HR
C      AMP ...PA
C
C      TRANSPORT MODEL
C      XK ...M/HR
C      XLAM...1/HR
C      R ...DIMENSIONLESS
C      D1 ...M**2/HR
C      D2 ...M
C
C      SOURCE MODEL
C      C0 ...ARBITRARY
C      ALPHA..1/HR
C
C      CONVERT FREQUENCY (1/HR) TO ANGULAR FREQUENCY (1/HR)
C      OMEGA=2.000*PI*F
C
C
C      20 NM1=N-1
C      DX=XL/DBLE(FLQAT(NM1))
C      NT=IFIX(SNGL(TMAX/DT))
C
C      F1=1.000/(R*DX*DX)
C      F2=1.000/(2.000*R*DX)
C      F3=F1/4.000
C
C      INITILIZE SOLUTE CONCENTRATION VECTOR
C      (AND ZERO OUT G MATRIX)
C      DO 10 K=1,N
C      C(K)=0.000
C      DO 5 J=1,5
C      G(J,K)=0.000
C      5 CONTINUE
C      10 CONTINUE
C

```

```

C      SET INITIAL SOURCE CONCENTRATION
C      C(1)=FUN(0.0)

C
C      COMMENCE TIME MARCH
C      DO 1000 J=1,NT
C      TIME=DBLE(FLOAT(J-1))*DT
C      T=TIME
C      XX(1,J)=T

C
C      ZERO OUT G(I,K), K=1,N
C      DO 40 K=1,N
C      G(1,K)=0.0D0
C 40 CONTINUE

C
C      I=2
C      COMMENCE RUNGE KUTTA SOLUTION
C 50 DO 100 K=2,NM1
C      X=DBLE(FLOAT(K-1))*DX

C
C      NOTE: X=0 IS THE LOCATION OF THE SOLUTE INJECTION POINT.
C      INCREASING X CORRESPONDS WITH DECREASING DEPTH.
C      X=XL IS THE SURFACE.
C
C      COMPUTE GAS VELOCITIES AT X-DX AND X+DX
C      FIRST MUST PUT DEPTHS IN REFERENCE FRAME OF FUNCTION VEL
C      DEPTH1=XL-(X-DX)
C      DEPTH2=XL-(X+DX)
C      DEPTH0=XL-X
C      VK =VEL(DEPTH0,T)
C      VKM1=VEL(DEPTH1,T)
C      VKP1=VEL(DEPTH2,T)

C
C      COMPUTE DISPERSION COEFFICIENTS
C      DK= D1+D2*DABS(VK)
C      DKM1=D1+D2*DABS(VKM1)
C      DKP1=D1+D2*DABS(VKP1)

C
C      BETA1= F1*DK+F2*VKM1-F3*(DKP1-DKM1)
C      BETA2=- (2.0D0*F1*DK+XLAM)
C      BETA3= F1*DK-F2*VKP1+F3*(DKP1-DKM1)

C
C      IF(K.EQ.NM1) GOTO 70
C      GOTO 80

C
C      APPLY DIFFERENT G(I,K) UPDATE FOR C(N-1)
C      .....
C
C 70 BOT=2.0D0*DX*(VKP1-VK)-3.0D0*DKP1
C      GAMNM2=DKP1/BOT
C      GAMNM1=-4.0D0*DKP1/BOT
C      G(I,K)= (BETA1+GAMNM2*BETA3)*(C(K-1)+G(I-1,K-1)/2.0D0)
C      X      +(BETA2+GAMNM1*BETA3)*(C(K) + G(I-1,K)/2.0D0)
C      G(I,K)=DT*G(I,K)
C      GOTO 100
C      .....

```

```

C
80 G(I,K)= BETA1*(C(K-1)+G(I-1,K-1)/2.0D0)
X      +BETA2*(C(K)  +G(I-1,K)  / 2.0D0)
X      +BETA3*(C(K+1)+G(I-1,K+1)/2.0D0)
      G(I,K)=DT*G(I,K)
C
100 CONTINUE
C
200 I=I+1
      IF(I.GT.5) GOTO 300
      IF(I.EQ.3.OR.I.EQ.4) T=TIME+DT/2.0D0
      IF(I.EQ.5) T=TIME+DT
      GOTO 50
C
C
C      UPDATE CONCENTRATION VECTOR TO NEW TIME
300 DQ 400 K=2,NM1
      C(K)=C(K)+(G(2,K)+2.0D0*(G(3,K)+G(4,K))+G(5,K))/5.0D0
400 CONTINUE
C
C      UPDATE C(1) AND C(N)
      VN=VEL(0.D0,T)
      C(1)=FUN(T)
C
      D=D1+D2*DABS(VN)
      TOP=D*C(N-2)-4.0D0*D*C(N-1)
      BOT=2.0D0*DX*(VN-XK)-3.0D0*D
      C(N)=TOP/BOT
C
C      ----- IDENTIFY SURFACE TRANSPORT PARAMETERS -----
C      COMPUTE CONCENTRATION GRADIENT AT X=XL
      GRAD=(C(N-2)-4.0*C(N-1)+3.0*C(N))/(2.0*DX)
C
C      FICKIAN FLUX (MOLECULAR DIFFUSION COMPONENT)
      B1=-SNGL(D*GRAD)
C
C      CONVECTIVE FLUX COMPONENT
      B2=SNGL(VN*C(N))
C
C      TOTAL SURFACE FLUX
      B3=SNGL(XK*C(N))
C
C      NOTE: B1 +B2 SHOULD = B3
C
      WRITE(*,*) SNGL(TIME),SNGL(C(N)),SNGL(VN)
      WRITE(*,*) B1,B2,B3
      WRITE(*,*)
C
C      OUTPUT SOLUTE FLUX AND PRESSURE HISTORY DATA TO DISK FILE.
C      NOTE: SOLUTE SURFACE FLUX IS SIMPLY VELOCITY x SOLUTE
C      CONCENTRATION. IF SOURCE CONCENTRATION IS IN KG/M**3, THEN
C      SURFACE FLUX IS IN (KG/M**2)/HR
C
      IF(MOD(J,NTOUT).NE.0) GOTO 800
      WRITE(21,*) SNGL(TIME),B1,B2,B3

```

```

      IF (MFLAG.EQ.0) WRITE(22,*) SNGL(TIME),SNGL(PRES)
C
      800 IF (MOD(J,NXOUT).NE.0) GOTO 1000
C      PLOT CONCENTRATION PROFILE AT GIVEN TIME
      DO 900 L=1,N
      XX(1,L)=FLOAT(L-1)*DX
      YY(1,L)=SNGL(C(L))
      900 CONTINUE
      PAUSE
      NPTS(1)=N
      CALL XPLOT(NPTS,1,ILINE,JLINE,XX,YY)
C
      1000 CONTINUE
C
C
      5000 FORMAT(' INPUT NAME OF DISK DATA FILE ',*)
      5010 FORMAT(A)
      5020 FORMAT(' INPUT NAME OF SOLUTE FLUX FILE ',*)
      5030 FORMAT(' INPUT NAME OF PRESSURE HISTORY FILE ',*)
      STOP
      END
      DOUBLE PRECISION FUNCTION VEL(X,T)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/ROCK/PAVG,DIFF,OMEGA,AMP,MFLAG,V
      COMMON/PRESS/PRES
C
C      VEL CALCULATES V(Z,T) FOR A HOMOGENEOUS AND ISOTROPIC HALF-
C      SPACE ASSUMING A SURFACE PRESSURE VARIATION OF THE FORM:
C
C      
$$P(0,T) = P_0 * \exp(i\omega t)$$

C
C      WHERE:  $\omega = 2\pi f$ ,  $f$  = FREQUENCY
C
C      /ROCK/ CONTAINS THE FOLLOWING SYSTEM PARAMETERS
C      PAVG ... AVERAGE FORMATION GAS PRESSURE (PA)
C      DIFF ... FORMATION DIFFUSIVITY (M**2/HR)
C      OMEGA... ANGULAR FREQUENCY OF SURFACE PRESSURE SIGNAL (1/HR)
C      AMP ... AMPLITUDE OF SURFACE PRESSURE SIGNAL (PA)
C
C      OPTIONAL MODEL:
C      IF (MFLAG.EQ.1), VELOCITY IS PRESCRIBED AND IS CONSTANT IN
C      SPACE AND TIME. THIS VELOCITY RESIDES IN COMMON/ROCK/ AS V.
C
C      NOTE ALSO THE PRESSURE VALUE FOR GIVEN X AND T IS RETURNED
C      IN COMMON/PRESS/
C
C      MODEL ASSUMES A HOMOGENEOUS AND ISOTROPIC HALF-SPACE WITH
C      A SURFACE PRESSURE SIGNAL OF THE FORM  $AMP * \exp(i * OMEGA * T)$ 
C      WHERE  $I = \sqrt{-1}$ 
C
C      RETURNED VELOCITY HAS UNITS OF M/HR
C
      NZED=0
      IF (MFLAG.EQ.NZED) GOTO 50
      VEL=V

```

```

      GOTO 100
C
50 ARG=DSQRT(OMEGA/(2.0D0*DIFF))
   FAC=DCOS(OMEGA*T-ARG*X)
   VEL=-AMP*(DIFF/PAVG)*ARG*DEXP(-ARG*X)*(DCOS(OMEGA*T-ARG*X)-
X                                           DSIN(OMEGA*T-ARG*X))
   PRES=AMP*DEXP(-ARG*X)*FAC
100 RETURN
   END
   DOUBLE PRECISION FUNCTION FUN(T)
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
   COMMON/SOURCE/C0,ALPHA
C
C   FUN CALCULATES THE SOURCE CONCENTRATION AS A FUNCTION OF TIME
C
   FUN=C0*DEXP(-ALPHA*T)
   RETURN
   END

```

```

C      ++++++
C      +////////////////////
C      +//////////////////// TRAN2 (Transport #2) //////////////////+
C      +////////////////////
C      ++++++
$DEBUG
$NOFLOATCALLS
$LARGE
      PROGRAM TRAN2

C
C      TRAN2 IS A 1-D CONVECTION-DIFFUSION MODEL THAT SOLVES
C      THE EQUATION:
C
C       $D*[d2C/dx2] - v*[dC/dx] - LAMBDA*R*C = R*[dC/dt]$ 
C
C      SUBJECT TO THE BOUNDARY CONDITIONS:
C
C      (A)       $-D*dC/dx + vC = KC, x=XL$ 
C
C      (B)       $C = C0*EXP(-ALPHA*T)$ 
C
C      PARAMETERS
C      C(X,T)      SOLUTE CONCENTRATION
C      D           SOLUTE DIFFUSIVITY
C      LAMBDA      SOLUTE DECAY RATE
C      R           RETARDATION FACTOR
C      v           SOLVENT VELOCITY (CONSTANT IN SPACE AND TIME)
C      K           SURFACE CONVECTION COEFFICIENT
C      C(0,T)      SOLUTE SOURCE TERM
C
C      METHOD OF SOLUTION:
C      THE D.E. + B.C.'S ARE SOLVED IN LAPLACE TRANSFORM SPACE AND
C      SUBSEQUENTLY TRANSFORMED BACK TO THE TIME DOMAIN USING A NUMERICAL
C      LAPLACE TRANSFORM INVERSION ALGORITHM.
C
C      WRITTEN BY:
C      JONATHAN M. HANSON
C      HANSON & ASSOCIATES
C      SALT LAKE CITY, UT
C      JULY, 1985
C
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C      IMPLICIT INTEGER*4 (I,J,K,L,M,N)
C      DIMENSION NPTS(2), ILINE(2), JLINE(2), XX(4,2000), YY(4,2000)
C      DIMENSION C(1000), V(20)
C
C      REAL*4 XX,YY
C      INTEGER*4 ONE
C      CHARACTER*20 FNAME, NTYPE
C      ONE=1
C
C      ----- INPUT MODEL AND CONTROL PARAMETERS -----
C      READ DATA FROM A DISK DATA FILE
C      WRITE(ID2,5000)
C      READ(ID1,5010) FNAME

```

```

      OPEN(20,FILE=FNAME, STATUS='OLD')
      READ(20,*) XL,TMAX
      READ(20,*) XK,XLAM,R,D1,D2,C0,VEL,ALPHA
      -----
C
C
C   PRESCRIBE NO. TERMS TO BE RETAINED IN INVERSE LAPLACE TRANSFORM
C   (NLAP IS ROUGHLY THE NUMBER OF SIGNIFICANT DIGITS RETAINED BY
C   THE COMPUTER...FOR AN IBM-PC IN DOUBLE PRECISION, THIS IS 12)
C   NLAP=12
C
      NX=100
      NT=100
      NPTS(1)=100
      NXM1=NX-1
      NTM1=NT-1
      DX=XL/FLOAT(NXM1)
      DT=TMAX/FLOAT(NTM1)
C
C   INITIALIZE NUMERICAL LAPLACE TRANSFORM INVERSION ARRAY
C   CALL LINV(NLAP,V)
C
C   COMPUTE EFFECTIVE DISPERSION COEFFICIENT
C   D=D1+D2*VEL
C
C   ZERO OUT ARRAYS
C   DO 5 J=1,1000
      XX(1,J)=0.0
      YY(1,J)=0.0
      C(J)=0.0
5   CONTINUE
C
C   SPECIFY EITHER COMPUTATIONS IN TIME OR SPACE
C   IF TIME, THEN THE CONCENTRATION HISTORY AT THE SURFACE IS
C   COMPUTED
C   IF SPACE, THEN THE CONCENTRATION PROFILE THROUGH THE SECTION
C   IS COMPUTED FOR THE SPECIFIED TIME
C
      WRITE(ID2,5020)
      READ(ID1,5010) NTYPE
C
      IF(NTYPE.EQ.'TIME') GOTO 10
      IF(NTYPE.EQ.'SPACE') GOTO 20
10  NX=1
      T0=0.0
      GOTO 50
C
20  NT=1
      WRITE(ID2,5030)
      READ(ID1,*) T0
C
C   BEGIN TIME MARCH
C   DO 1010 J=1,NT
      T=FLOAT(J-1)*DT+T0
      IF(T.EQ.0.0) GOTO 1010
C

```

```

60 AB=DLOG(2.0D0)/T
C
      DO 1000 K=1,NX
C
      IF (NTYPE.EQ.'SPACE') X=FLOAT(K-1)*DX
      IF (NTYPE.EQ.'TIME') X=XL
C
      IF (NTYPE.EQ.'TIME') XX(1,J)=T
      IF (NTYPE.EQ.'SPACE') XX(1,K)=X
C
C *****
C COMMENCE NUMERICAL LAPLACE TRANSFORM INVERSION
C SUM=0.0
      DO 500 KK=1,NLAP
      S=FLOAT(KK)*AB
C
      FUN=C0/S
      IF (X.EQ.0.0) GOTO 400
C
      ARG=DSQRT((VEL/D)**2+4.0*((R/D)*(XLAM+S)))
      BPL=((VEL/D)+ARG)/2.0
      BMI=((VEL/D)-ARG)/2.0
      FPX=DEXP(BPL*X)
      FMX=DEXP(BMI*X)
      FPXL=DEXP(BPL*XL)
      FMXL=DEXP(BMI*XL)
C
      XI1=-D*BPL*FPXL+(VEL-XK)*FPXL
      XI2=-D*BMI*FMXL+(VEL-XK)*FMXL
C
      FUN=(XI2*FPX-XI1*FMX)/(XI2-XI1)
      FUN=FUN*C0/(S+ALPHA)
C
400      SUM=SUM+V(KK)*FUN
500      CONTINUE
      SUM=SUM*AB
C *****
C
600      IF (NTYPE.EQ.'TIME') C(J)=SUM
      IF (NTYPE.EQ.'SPACE') C(K)=SUM
C
      IF (NTYPE.EQ.'TIME') YY(1,J)=SUM
      IF (NTYPE.EQ.'SPACE') YY(1,K)=SUM
C
      IF (NTYPE.EQ.'TIME') WRITE(*,*) T,C(J)
      IF (NTYPE.EQ.'SPACE') WRITE(*,*) X,C(K)
C
1000      CONTINUE
1010 CONTINUE
C
      ILINE(1)=1
      JLINE(1)=7
      CALL XPLOT(NPTS,ONE,ILINE,JLINE,XX,YY)
C
5000 FORMAT(' INPUT NAME OF DISK DATA FILE ',*)

```



```

5010 FORMAT(A)
5020 FORMAT(' TIME OR SPACE? ', $)
5030 FORMAT(' SPECIFY TIME? ', $)
STOP
END
SUBROUTINE LINV(N,V)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
IMPLICIT INTEGER*4 (I,J,K,L,M,N)
DIMENSION V(1),G(100),H(100)
C
C LINV COMPUTES THE SUMMATION COEFFICIENTS USED IN THE INVERSE
C LAPLACE TRANSFORM.
C
G(1)=1.0
NH=N/2
DO 100 I=1,N
G(I+1)=G(I)*FLOAT(I)
100 CONTINUE
H(1)=2.0/G(NH)
DO 200 I=2,NH
H(I)=(FLOAT(I)**NH)*G(2*I+1)/(G(NH-I+1)*G(I+1)*G(I))
200 CONTINUE
SN=2.0*FLOAT(MOD(NH,2))-1.0
DO 400 I=1,N
V(I)=0.0
NTOP=MIN0(I,NH)
NBOT=(I+1)/2
DO 300 K=NBOT,NTOP
V(I)=V(I)+H(K)/(G(I-K+1)*G(2*K-I+1))
300 CONTINUE
V(I)=SN*V(I)
SN=-SN
400 CONTINUE
RETURN
END

```

TIME DOMAIN CODE MODELS - CHIMNEY ANALYSIS

(LINK WITH DRIVER1)

C)

```

$!LARGE
$NOFLOATCALLS
$DEBUG
C
C
C      ++++++
C      +//
C      +// TDCMOD1 //
C      +//
C      ++++++
C
C      TDCMOD1 - TIME DOMAIN CHIMNEY MODEL #1
C
C      TDCMOD1 ASSUMES A HOMOGENEOUS AND ISOTROPIC HALF-SPACE WITH A
C      SINGLE PRESSURE SENSOR DEPLOYED AT A GIVEN DEPTH
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = DEPTH TO PRESSURE SENSOR (M)
C      B(3) = INITIAL (T=0) DOWNHOLE (IN-CHIMNEY) PRESSURE
C
C      FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(1),A(1),B(10),TEMP(20),V(20)
C      COMMON/STUFF/XINP(2000),YINP(2000),G(2000),NPTS,NLAP,V
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C      DT=X(2)-X(1)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=A(K)
C      5 CONTINUE
C
C      G(1)=0.0
C      IF(1.GT.1) GOTO 100
C
C      CALCULATE IMPULSE RESPONSE G IN THE TIME DOMAIN
C      DO 50 J=2,NPTS
C      ARG=SQRT(B(2)*B(2)/(4.0*B(1)*DT*FLOAT(J)))
C      G(J)=1.0-ERF(ARG)
C      50 CONTINUE
C
C      CONVOLVE IMPULSE RESPONSE WITH SYSTEM INPUT
C      100 SUM=0.0
C      YINP(NPTS+1)=YINP(NPTS)
C      DO 200 J=1,I
C      M=I-J+1
C      SUM=SUM+G(M)*(YINP(J+1)-YINP(J))
C      200 CONTINUE
C      FUNCTN=SUM+B(3)
C      RETURN
C      END
C      FUNCTION ERF(X)
C      ERROR FUNCTION...SEE ABROMOWITZ AND STEGUN, P. 299

```

```

ERF=1.0
ARG=X*X
IF(ARG.GT.20.0) GOTO 10
P= 0.3275911
A1= 0.254829592
A2=-0.284496736
A3= 1.421413741
A4=-1.453152027
A5= 1.061405429
T=1.0/(1.0+P*X)
F1=A1+T*(A2+T*(A3+T*(A4+T*A5)))
F1=T*F1
ERF=1.0-F1*EXP(-ARG)
10 RETURN
END

```

```

$LARGE
$NOFLOATCALLS
$DEBUG
C
C
C      ++++++
C      +////////////////////
C      +//////////////////// TDCMOD2 //////////////////////
C      +////////////////////
C      ++++++
C
C      TDCMOD2 - TIME DOMAIN CHIMNEY MODEL #2
C
C      TDCMOD2 ASSUMES A HOMOGENEOUS AND ISOTROPIC FORMATION WITH A "NO-
C      FLOW" BOUNDARY AT A PRESCRIBED DEPTH. A SINGLE PRESSURE IS
C      DEPLOYED AT A PRESCRIBED DEPTH. CALCULATIONS INVOLVE A NUMERICAL
C      LAPLACE TRANSFORM INVERSION.
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = DEPTH TO PRESSURE SENSOR (M)
C      B(3) = CHIMNEY DEPTH (M) (ALSO, DEPTH TO "NO FLOW" BOUNDARY)
C
C      FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(1),A(1),B(10),TEMP(20),V(20)
C      COMMON/STUFF/XINP(2000),YINP(2000),G(2000),NPTS,NLAP,V
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C
C      DT=X(2)-X(1)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=A(K)
C      5 CONTINUE
C
C
C      G(1)=0.0
C      IF(I.GT.1) GOTO 100
C
C      CALCULATE IMPULSE RESPONSE G IN THE TIME DOMAIN
C      DO 50 J=2,NPTS
C      T=FLOAT(J-1)*DT
C      AB=ALOG(2.0)/T
C
C      DO 30 KK=1,NLAP
C      S=FLOAT(KK)*AB
C      S IS THE LAPLACE TRANSFORM VARIABLE CORRESPONDING TO TIME.
C
C      ARG1=SQRT(S/B(1))*B(2)
C      ARG2=SQRT(S/B(1))*2.0*B(3)
C
C      IF(ARG2.GT.20) FAC2=0.0
C      IF(ARG2.LE.20) FAC2=EXP(-ARG2)
C

```

```

TOP=EXP(-ARG1)+FAC2*EXP(ARG1)
BOT=1.0+FAC2

C
PHOMOG=TOP/BOT

C
C ADD SUMMATION AND HOMOGENEOUS SOLUTIONS
20 TEMP(KK)=PHOMOG
30 CONTINUE

C
C COMPUTE LAPLACE INVERSE FOR CURRENT TIME VALUE
SUM2=0.0
DO 40 KK=1,NLAP
SUM2=SUM2+V(KK)*TEMP(KK)
40 CONTINUE
G(J)=AB*SUM2*DT
50 CONTINUE

C
C CONVOLVE IMPULSE RESPONSE WITH SYSTEM INPUT
100 SUM=0.0
YINP(NPTS+1)=YINP(NPTS)
DO 200 J=1,I
SUM=SUM+G(J)*(YINP(I-J+1)+YINP(I-J+2))/2.0
200 CONTINUE
FUNCTN=SUM
RETURN
END
SUBROUTINE LINV(N,V)
DIMENSION V(20),G(100),H(100)

C
G(1)=1.0
NH=N/2
DO 100 I=1,N
G(I+1)=G(I)*FLOAT(I)
100 CONTINUE
H(1)=2.0/G(NH)
DO 200 I=2,NH
H(I)=(FLOAT(I)**NH)*G(2*I+1)/(G(NH-I+1)*G(I+1)*G(I))
200 CONTINUE
SN=2.0*FLOAT(MOD(NH,2))-1.0
DO 400 I=1,N
V(I)=0.0
NTOP=MIN0(I,NH)
NBOT=(I+1)/2
DO 300 K=NBOT,NTOP
V(I)=V(I)+H(K)/(G(I-K+1)*G(2*K-I+1))
300 CONTINUE
V(I)=SN*V(I)
SN=-SN
400 CONTINUE
RETURN
END

```

```

$LARGE
$NOFLOATCALLS
$DEBUG
C *****
C +//////////////////////////////////////////////////////////////////+
C +////////////////////////////////////////////////////////////////// TDCMOD3 //+
C +//////////////////////////////////////////////////////////////////+
C *****
C
C TDCMOD3 - TIME DOMAIN CHIMNEY MODEL #3
C
C TDCMOD3 ASSUMES A HOMOGENEOUS AND ISOTROPIC HALF-SPACE WITH A
C SINGLE PRESSURE TRANSDUCER DEPLOYED AT A PRESCRIBED DEPTH IN
C A PARTIALLY CASSED BUT OTHERWISE OPEN HOLE. THE COMPUTED PRESSURE
C IS BASED ON A VERTICAL AVERAGE OF THE 1-D FLOW MODEL OVER THE
C OPEN HOLE SECTION. (SEE HANSON, UCRL 15699, 1984).
C
C MODEL PARAMETERS:
C B(1) = CASING LENGTH (M)
C B(2) = HOLE DEPTH (M)
C B(3) = DIFFUSIVITY (M**2/HR)
C
C FUNCTION FUNCTN(X,I,A)
C DIMENSION X(1),A(1),B(10)
C
C COMMON /STUFF/XINP(2000),YINP(2000),G(2000),NPTS
C COMMON /ZAP/JFR(10),NTERMS,NFR
C
C DT=X(2)-X(1)
C PI=3.14159265
C
C DECODE PARAMETERS
C DO 10 K=1,NTERMS
C B(JFR(K))=A(K)
10 CONTINUE
C
C IF(1.GT.1) GOTO 25
C CALCULATE IMPULSE RESPONSE IN THE TIME DOMAIN
C ARG1=B(1)**2/(4.0*B(3))
C ARG2=B(2)**2/(4.0*B(3))
C DO 20 J=1,NPTS
C T=FLOAT(J-1)*DT
C
C G(J)=EXP(-ARG1/T)-EXP(-ARG2/T)
C G(J)=(1.0/(B(2)-B(1)))*SQRT(B(3)/(PI*T))*G(J)
C
C T1=T
C T2=T+DT
C
C IF(T.GT.0.0) GOTO 15
C F1=SQRT(T2)*EXP(-ARG1/T2)
C F2=SQRT(T2)*EXP(-ARG2/T2)
C G1=SQRT(PI*ARG1)*(ERF(SQRT(ARG1/T2))-1.0)

```

```

G2=SQRT(PI*ARG2)*(ERF(SQRT(ARG2/T2))-1.0)
G(J)=(2.0/(B(2)-B(1)))*SQRT(B(3)/PI)*(F1-F2+G1-G2)
GOTO 20

C
15 F1=SQRT(T2)*EXP(-ARG1/T2)-SQRT(T1)*EXP(-ARG1/T1)
F2=SQRT(T2)*EXP(-ARG2/T2)-SQRT(T1)*EXP(-ARG2/T1)
G1=SQRT(PI*ARG1)*(ERF(SQRT(ARG1/T2))-ERF(SQRT(ARG1/T1)))
G2=SQRT(PI*ARG2)*(ERF(SQRT(ARG2/T2))-ERF(SQRT(ARG2/T1)))
G(J)=(2.0/(B(2)-B(1)))*SQRT(B(3)/PI)*(F1-F2+G1-G2)
20 CONTINUE

C
C CONVOLVE IMPULSE RESPONSE WITH SYSTEM INPUT
25 SUM=0.0
YINP(NPTS+1)=YINP(NPTS)
DO 30 J=1,I
SUM=SUM+G(J)*(YINP(I-J+1)+YINP(I-J+2))/2.0
30 CONTINUE
FUNCTN=SUM
RETURN
END
FUNCTION ERF(X)
C ERROR FUNCTION...SEE ABROMOWITZ AND STEGUN, P. 299
ERF=1.0
ARG=X*X
IF(ARG.GT.20.0) GOTO 10
P= 0.3275911
A1= 0.254829592
A2=-0.284496736
A3= 1.421413741
A4=-1.453152027
A5= 1.061405429
T=1.0/(1.0+P*X)
F1=A1+T*(A2+T*(A3+T*(A4+T*A5)))
F1=T*F1
ERF=1.0-F1*EXP(-ARG)
GOTO 20
10 ERF=1.0
20 RETURN
END

```



```

#LARGE
#NOFLOATCALLS
#DEBUG
C
C
C      ++++++
C      +/////////////////////////
C      +///////////////////////// TDCMOD4 ///////////////////////////
C      +/////////////////////////
C      ++++++
C
C      TDCMOD4 - TIME DOMAIN CHIMNEY MODEL 4
C
C      TDCMOD4 ASSUMES A HOMOGENEOUS AND ISOTROPIC FORMATION WITH A "NO-
C      FLOW" BOUNDARY AT A PRESCRIBED DEPTH. A SINGLE SUBSURFACE
C      PRESSURE TRANSDUCER IS DEPLOYED IN A PARTIALLY CASED, BUT
C      OTHERWISE OPEN, HOLE. THE 1-D VERTICAL AVERAGE APPROXIMATION
C      IS USED (SEE HANSON, UCRL 15699, 1984). A NUMERICAL LAPLACE
C      TRANSFORM INVERSION IS USED IN THE CALCULATION.
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = CHIMNEY DEPTH (M) (ALSO, DEPTH TO "NO FLOW" BOUNDARY)
C      B(3) = CASING LENGTH ON SENSING HOLE
C      B(4) = SENSING HOLE DEPTH
C
C
C      FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(1),A(1),B(10),TEMP(20),V(20)
C      COMMON/STUFF/XINP(2000),YINP(2000),B(2000),NPTS,NLAP,V
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C      DOUBLE PRECISION B,TEMP,ARG1,ARG2,ARG3,PHOMOG,S,TOP,BOT
C      DOUBLE PRECISION V,SUM2
C
C
C      DT=X(2)-X(1)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=DBLE(A(K))
C 5 CONTINUE
C
C
C      G(1)=0.0
C      IF(I.GT.1) GOTO 100
C
C      CALCULATE IMPULSE RESPONSE G IN THE TIME DOMAIN
C      DO 50 J=2,NPTS
C      T=FLOAT(J-1)*DT
C      AB=ALOG(2.0)/T
C
C      DO 30 KK=1,NLAP
C      S=DBLE(FLOAT(KK)*AB)
C      S IS THE LAPLACE TRANSFORM VARIABLE CORRESPONDING TO TIME.
C
C      ARG1=DSQRT(S/B(1))*(B(4)-B(2))

```

```

      ARG2=DSQRT(S/B(1))*(B(3)-B(2))
      ARG3=DSQRT(S/B(1))*B(2)
C
      TOP=DSINH(ARG1)-DSINH(ARG2)
      BOT=DCOSH(ARG3)
C
C
      PHOMOG=(1.0D0/(B(4)-B(3)))*DSQRT(B(1)/S)*TOP/BOT
C
C      ADD SUMMATION AND HOMOGENEOUS SOLUTIONS
20  TEMP(KK)=PHOMOG
30  CONTINUE
C
C      COMPUTE LAPLACE INVERSE FOR CURRENT TIME VALUE
      SUM2=0.0D0
      DO 40 KK=1,NLAP
      SUM2=SUM2+V(KK)*TEMP(KK)
40  CONTINUE
      G(J)=AB*SNGL(SUM2)*DT
50  CONTINUE
C
C      CONVOLVE IMPULSE RESPONSE WITH SYSTEM INPUT
100 SUM=0.0
      YINP(NPTS+1)=YINP(NPTS)
      DO 200 J=1,I
      SUM=SUM+DT*G(J)*(YINP(I-J+1)+YINP(I-J+2))/2.0
200 CONTINUE
      FUNCTN=SUM
      RETURN
      END
      SUBROUTINE LINV(N,V)
      DIMENSION V(20),G(100),H(100)
      DOUBLE PRECISION V,G,H,SN
C
      G(1)=1.0D0
      NH=N/2
      DO 100 I=1,N
      G(I+1)=G(I)*DBLE(FLOAT(I))
100 CONTINUE
      H(1)=2.0D0/G(NH)
      DO 200 I=2,NH
      H(I)=(DBLE(FLOAT(I))*NH)*G(2*I+1)/(G(NH-I+1)*G(I+1)*G(I))
200 CONTINUE
      SN=2.0D0*DBLE(FLOAT(MOD(NH,2)))-1.0)
      DO 400 I=1,N
      V(I)=0.0D0
      NTOP=MIN0(I,NH)
      NBOT=(I+1)/2
      DO 300 K=NBOT,NTOP
      V(I)=V(I)+H(K)/(G(I-K+1)*G(2*K-I+1))
300 CONTINUE
      V(I)=SN*V(I)
      SN=-SN
400 CONTINUE
      RETURN

```

END

```

$LARGE
$NOFLOATCALLS
$DEBUG
C
C
C      ++++++
C      ++++++
C      ++++++ TDCMODS ++++++
C      ++++++
C      ++++++
C
C      TDCMODS - TIME DOMAIN CHIMNEY MODEL #5
C
C      TDCMODS ASSUMES A HOMOGENEOUS AND ISOTROPIC CHIMNEY OF CONSTANT
C      DIAMETER IS CONTAINED WITHIN A HOMOGENEOUS AND ISOTROPIC FORMATION
C      OF DIFFERENT GAS FLOW PROPERTIES. THE MODEL ASSUMES THERE EXISTS
C      A NO-FLOW BOUNDARY AT A PRESCRIBED DEPTH AND THAT THE BASE OF THE
C      CHIMNEY IS AT THIS DEPTH. A NUMERICAL LAPLACE TRANSFORM INVERSION
C      IS USED IN THE CALCULATION.
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = FORMATION DIFFUSIVITY (M**2/HR)
C      B(3) = FORMATION PERMEABILITY/CHIMNEY PERMEABILITY (DIMENSIONLESS)
C      B(4) = DEPTH TO PRESSURE SENSOR (M)
C      B(5) = CHIMNEY RADIUS (M)
C      B(6) = CHIMNEY DEPTH (M) (ALSO, DEPTH TO "NO FLOW" BOUNDARY)
C      B(7) = INITIAL (T=0) PRESSURE
C
C      FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(1),A(1),B(10),TEMP(20)
C      DOUBLE PRECISION V(20)
C      COMMON/STUFF/XINP(2000),YINP(2000),G(2000),NPTS,NLAP,V,EPS
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C
C      DT=X(2)-X(1)
C      PI=3.14159265
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=A(K)
C 5 CONTINUE
C
C
C      G(1)=0.0
C      IF(I.GT.1) GOTO 100
C
C      CALCULATE IMPULSE RESPONSE G IN THE TIME DOMAIN
C      DO 50 J=2,NPTS
C      T=FLOAT(J-1)*DT
C      AB=ALOG(2.0)/T
C
C      DO 30 KK=1,NLAP
C      S=FLOAT(KK)*AE

```

```

C      S IS THE LAPLACE TRANSFORM VARIABLE CORRESPONDING TO TIME.
C
      SUM=0.0
      N=0
      NMAX=-1
      IF (B(1).EQ.B(2)) GOTO 18
C
      10 BN=(N+0.5)*PI/B(6)
      BETA=SQRT(BN*BN+S/B(2))
      GAMM=SQRT(BN*BN+S/B(1))
      F1=BETA*BETA*B(2)
      F2=GAMM*GAMM*B(1)
      ARG1=BETA*B(5)
      ARG2=GAMM*B(5)
      A1=BETA*BETA*GAMM*GAMM
C
      CONSTRUCT BESJ0(ARG2)/BESJ1(ARG2) FOR LARGE ARGUMENTS
      IF (ARG2.GT.10.) RAT=(ARG2*(ARG2*(ARG2+0.125)+0.0703125)+0.0732422)
X      / (ARG2*(ARG2*(ARG2-0.375)-0.1171875)-0.1025391)
C
      IF (ARG2.LE.10.) RAT=BESJ0(ARG2)/BESJ1(ARG2)
C
      BOT=A1*(1.0+B(3))*RAT*(BETA*BESK1(ARG1))/
X      (GAMM*BESK0(ARG1))
      TOP=BN*SIN(BN*B(4))
C
      DELTA=(B(1)-B(2))*TOP/(F1*F2*BOT)
      IF (N.LT.5) GOTO 15
C
      CHECK FOR SUMMATION CONVERGENCE
      IF (ABS(DELTA/SUM).LT.EPS) GOTO 18
      15 IF (N.GT.500) GOTO 18
      SUM=SUM+DELTA
      N=N+1
      GOTO 10
C
      COMPUTE HOMOGENEOUS SOLUTION
      18 ARG3=SQRT(S/B(2))*B(4)
      ARG4=SQRT(S/B(2))*B(6)
      PHOMDG=(EXP(ARG3)+EXP(2.0*ARG4)*EXP(-ARG3))/
X      (1.0+EXP(2.0*ARG4))
C
      ADD SUMMATION AND HOMOGENEOUS SOLUTIONS
      20 TEMP(KK)=(2.0/B(6))*S*SUM+PHOMDG
      IF (N.GT.NMAX) NMAX=N
      30 CONTINUE
C
      COMPUTE LAPLACE INVERSE FOR CURRENT TIME VALUE
      SUM2=0.0
      DO 40 KK=1,NLAP
      SUM2=SUM2+V(KK)*TEMP(KK)
      40 CONTINUE
      G(J)=AB*SUM2*DT
      WRITE(*,*) J,NMAX,G(J)
      50 CONTINUE

```

```

C
C      CONVOLVE IMPULSE RESPONSE WITH SYSTEM INPUT
100 SUM=0.0
      YINP(NPTS+1)=YINP(NPTS)
      DO 200 J=1,I
        SUM=SUM+B(J)*(YINP(I-J+1)+YINP(I-J+2))/2.0
200 CONTINUE
      FUNCTN=SUM+B(7)
      RETURN
      END
      FUNCTION BESK0(X)
      A1=-0.57721566
      A2=0.42278420
      A3=0.23069756
      A4=0.03488590
      A5=0.00262698
      A6=0.00010750
      A7=0.00000740

C
      B1=1.25331414
      B2=-0.07832358
      B3=0.02189568
      B4=-0.01062446
      B5=0.00587872
      B6=-0.00251540
      B7=0.00053208

C
      IF(X.GT.2.0) GOTO 10
      R=(X/2.0)**2
      F=R*(A2+R*(A3+R*(A4+R*(A5+R*(A6+R*A7))))
      BESK0=-ALOG(X/2.0)*BESJ0(X)+A1+F
      RETURN
10 R=2.0/X
      F=R*(B2+R*(B3+R*(B4+R*(B5+R*(B6+R*B7))))
      BESK0=EXP(-X)*(B1+F)/SQRT(X)
      RETURN
      END
      FUNCTION BESK1(X)
      A1=0.15443144
      A2=-0.67278579
      A3=-0.18156897
      A4=-0.01919402
      A5=-0.00110404
      A6=-0.00004686

C
      B1=1.25331414
      B2=0.23498619
      B3=-0.03655620
      B4=0.01504268
      B5=-0.00780353
      B6=0.00325614
      B7=-0.00068245

C
      IF(X.GT.2.0) GOTO 10
      R=(X/2.0)**2

```

```

F=R*(A1+R*(A2+R*(A3+R*(A4+R*(A5+R*A6))))
BESK1=(1.0+F*X*ALOG(X/2.0)*BESI1(X))/X
RETURN
10 R=2.0/X
F=R*(B2+R*(B3+R*(B4+R*(B5+R*(B6+R*B7))))
BESK1=(B1+F)*EXP(-X)/SQRT(X)
RETURN
END
FUNCTION BESI0(X)
A1=3.5156229
A2=3.0899424
A3=1.2067492
A4=0.2659732
A5=0.0360768
A6=0.0045813
C
B1=0.39894228
B2=0.01328592
B3=0.00225319
B4=-0.00157565
B5=0.00916821
B6=-0.02057706
B7=0.02635537
B8=-0.01647633
B9=0.00392377
C
T=X/3.75
IF(X.GT.3.75) GOTO 10
R=T*T
F=R*(A1+R*(A2+R*(A3+R*(A4+R*(A5+R*A6))))
BESI0=1.0+F
RETURN
10 R=1.0/T
F=R*(B2+R*(B3+R*(B4+R*(B5+R*(B6+R*(B7+R*(B8+R*B9))))))
BESI0=EXP(X)*(B1+F)/SQRT(X)
RETURN
END
FUNCTION BESI1(X)
A1=0.87890594
A2=0.51498869
A3=0.15084934
A4=0.02658733
A5=0.00301532
A6=0.00032411
C
B1=0.39894228
B2=-0.03988024
B3=-0.00362018
B4=0.00163801
B5=-0.01031555
B6=0.02282967
B7=-0.02695312
B8=0.01787654
B9=-0.00420059
C

```

```

T=X/3.75
IF(X.GT.3.75) GOTO 10
R=T*T
F=R*(A1+R*(A2+R*(A3+R*(A4+R*(A5+R*A6))))
BESI1=(0.5+F)*X
RETURN
10 R=1.0/T
F=R*(B2+R*(B3+R*(B4+R*(B5+R*(B6+R*(B7+R*(B8+R*B9))))))
BESI1=EXP(X)*(B1+F)/SQRT(X)
RETURN
END
SUBROUTINE LINV(N,V)
DIMENSION G(100),H(100)
DOUBLE PRECISION V(20)
C
G(1)=1.0
NH=N/2
DO 100 I=1,N
G(I+1)=G(I)*FLOAT(I)
100 CONTINUE
H(1)=2.0/G(NH)
DO 200 I=2,NH
H(I)=(FLOAT(I)**NH)*G(2*I+1)/(G(NH-I+1)*G(I+1)*G(I))
200 CONTINUE
SN=2.0*FLOAT(MOD(NH,2))-1.0
DO 400 I=1,N
V(I)=0.0
NTOP=MIN0(I,NH)
NBOT=(I+1)/2
DO 300 K=NBOT,NTOP
V(I)=V(I)+H(K)/(G(I-K+1)*G(2*K-I+1))
300 CONTINUE
V(I)=SN*V(I)
SN=-SN
400 CONTINUE
RETURN
END

```


FREQUENCY DOMAIN CODE MODULES

(LINK WITH DRIVER2)

```

$LARGE
$NOFLOATCALLS
$DEBUG

```

```

C
C      ++++++
C      +////////////////////
C      +//////////////////// FDCMOD1 //////////////////////
C      +////////////////////
C      ++++++
C
C      FDCMOD1 - FREQUENCY DOMAIN CHIMNEY MODEL #1
C
C      FDCMOD1 ASSUMES A HOMOGENEOUS AND ISOTROPIC HALF-SPACE. A SINGLE
C      DOWNHOLE PRESSURE TRANSDUCER IS DEPLOYED IN A PARTIALLY CASED
C      BUT OTHERWISE OPEN HOLE. THE 1-D VERTICAL AVERAGE APPROXIMATION
C      IS MADE. (SEE HANSON, UCRL 15699, 1984). THE IN-HOLE AMPLITUDE
C      SPECTRUM IS COMPUTED ON THE BASIS OF THE SURFACE AMPLITUDE
C      SPECTRUM (INPUT) AND THE SYSTEM TRANSFER FUNCTION (COMPUTED).
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = LENGTH OF SENSING HOLE CASING (M)
C      B(3) = LENGTH OF SENSING HOLE
C
C      AMPLITUDE SPECTRUM ONLY
C      COMPLEX FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(1),A(1),B(10)
C      COMMON/STUFF/XINP(2000),YINP(2000),NPTS
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C      TWOPI=6.283185308
C
C      DX=X(2)-X(1)
C
C      XI=CMPLX(0.0,1.0)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=A(K)
C      S CONTINUE
C
C
C      OMEGA=TWOPI*FLOAT(I-1)*DX+X(1)
C      IF(OMEGA,NE.0.0) GOTO 10
C      FAC=1.0
C      GOTO 20
C 10 ARG=OMEGA/(2.0*B(1))
C      SQARG=SQRT(ARG)
C      FAC=(EXP(-B(3)*SQARG)-EXP(-B(2)*SQARG))/SQARG
C      FAC=-FAC/(B(3)-B(2))
C 20 FUNCTN=FAC*YINP(I)
C      RETURN
C      END

```

```

$LARGE
$NOFLOATCALLS
$DEBUG
C
C
C      ++++++
C      +//
C      +// FDCMOD2 //
C      +//
C      ++++++
C
C      FDCMOD2 - FREQUENCY DOMAIN CHIMNEY MODEL 2
C
C      FDCMOD2 ASSUMES A HOMOGENEOUS AND ISOTROPIC HALF-SPACE AND USES
C      THE VERTICAL AVERAGE APPROXIMATION (SEE HANSON, UCRL 15639,
C      1984). THE REAL AND IMAGINARY PARTS
C      OF THE COMPUTED DOWNHOLE PRESSURE (IN THE FREQUENCY DOMAIN) ARE
C      COMPUTED ON THE BASIS OF THE REAL AND IMAGINARY PARTS OF THE
C      SURFACE PRESSURE AND THE COMPUTED TRANSFER FUNCTION.
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = LENGTH OF SENSING HOLE CASING (M)
C      B(3) = LENGTH OF SENSING HOLE
C
C      COMPLEX FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(500),A(10)
C      COMPLEX YINP(500),XI,FAC,ARG,B(10),COMEGA,SGARG
C      COMMON/STUFF/XINP(500),YINP,NPTS
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C      TWOPI=6.283185306
C      DX=X(2)-X(1)
C      XI=CMPLX(0.0,1.0)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=CMPLX(A(K),0.0)
C      5 CONTINUE
C
C
C      OMEGA=TWOPI*FLOAT(I-1)*DX+X(1)
C      COMEGA=CMPLX(OMEGA,0.0)
C      IF(OMEGA.NE.0.0) GOTO 10
C      FAC=CMPLX(1.0,0.0)
C      GOTO 20
C
C      10 ARG=XI*COMEGA/B(1)
C      SGARG=CSQRT(ARG)
C      FAC=(CEXP(-B(3)*SGARG)-CEXP(-B(2)*SGARG))/SGARG
C      FAC=-FAC/(B(3)-B(2))
C      20 FUNCTN=FAC*YINP(I)
C      RETURN
C      END

```

```

$LARGE
$NOFLOATCALLS
$DEBUG
C
C      ++++++
C      +////////////////////-
C      +//////////////////// FDCMOD3 //////////////////-
C      +////////////////////-
C      ++++++
C
C      FDCMOD3 - FREQUENCY DOMAIN CHIMNEY MODEL #3
C
C      FDCMOD3 ASSUMES A HOMOGENEOUS AND ISOTROPIC FORMATION WITH A "NO-
C      FLOW" BOUNDARY AT A PRESCRIBED DEPTH. THE 1-D VERTICAL AVERAGE
C      APPROXIMATION IS MADE (SEE HANSON, UCRL 15699, 1984). A SINGLE
C      DOWNHOLE PRESSURE TRANSDUCER IS DEPLOYED IN A PARTIALLY CASED,
C      BUT OTHERWISE OPEN, HOLE. THE REAL AND IMAGINARY PARTS OF THE
C      IN-HOLE PRESSURE RESPONSE ARE COMPUTED ON THE BASIS OF THE REAL
C      AND IMAGINARY PARTS OF THE SURFACE PRESSURE AND THE COMPUTED
C      TRANSFER FUNCTION.
C
C      MODEL PARAMETERS:
C      B(1) = CHIMNEY DIFFUSIVITY (M**2/HR)
C      B(2) = LENGTH OF SENSING HOLE CASING (M)
C      B(3) = LENGTH OF SENSING HOLE
C      B(4) = DEPTH TO NO-FLOW BOUNDARY
C
C      COMPLEX FUNCTION FUNCTN(X,I,A)
C      DIMENSION X(500),A(10),B(10)
C      COMPLEX YINP(500),XI,ARG,SQARG, TOP, BOT
C      COMPLEX FAC1A,FAC1B,FAC2A,FAC2B,FACA,FACB,FAC
C      COMMON/STUFF/XINP(500),YINP,NPTS
C      COMMON/ZAP/JFR(10),NTERMS,NFR
C
C      TWOPI=6.283185308
C      DX=X(2)-X(1)
C      XI=CMPLX(0.0,1.0)
C
C      DECODE PARAMETERS
C      DO 5 K=1,NTERMS
C      B(JFR(K))=A(K)
C      5 CONTINUE
C
C      OMEGA=TWOPI*(FLOAT(I-1)*DX+X(1))
C      IF (OMEGA.NE.0.0) GOTO 10
C      FAC=CMPLX(1.0,0.0)
C      GOTO 20
C
C      10 ARG=XI*OMEGA/B(1)
C      SQARG=CSQRT(ARG)
C      FAC1A=+CEXP(-B(3)*SQARG)
C      FAC1B=-CEXP(-B(2)*SQARG)
C      FAC2A=+CEXP(+B(3)*SQARG)
C      FAC2B=-CEXP(+B(2)*SQARG)
C      FACA=CEXP(+B(4)*SQARG)

```

```

FACB=CEXP(-B(4)*SQARG)
TOP=FACA*(FAC1A+FAC1B)+FACB*(FAC2A+FAC2B)
BOT=(B(3)-B(2))*SQARG*(FACA-FACB)
FAC=-TOP/BOT
20 FUNCTN=FAC*YINP(I)
RETURN
END

```

```

C      ++++++
C      ++++++
C      ++++++ RCHAN (Run Chimney ANalysis) ++++++
C      ++++++
C      ++++++
C
C      WRITTEN BY:
C      JONATHAN M. HANSON
C      HANSON & ASSOCIATES
C      SALT LAKE CITY, UT 84108
C      AUGUST, 1985
C
C      BASED ON: PRICKETT, T.A. AND LONNQUIST, C.G., "SELECTED DIGITAL
C      COMPUTER TECHNIQUES FOR GROUNDWATER RESOURCE EVALUATION",
C      BULLETIN 55, ILLINOIS STATE WATER SURVEY, URBANA
C
C      APPLICATION:
C      RCHAN SETS UP REQUIRED DATA FILES FOR INPUT INTO THE
C      PROGRAM "CHAN" AND "FCHAN"
C
C      $DEBUG
C      $NOFLOATCALLS
C      $LARGE
C          DIMENSION C(20,200,2),SF(20,200),P(20,200),Q(20,200),
X      RC(20),ZC(200),PERM(10),POR(10),THICKL(10),NV(10),
X      PERM2(10),POR2(10)
C          CHARACTER*20 OUTPUT
C          PI=3.141592654
C          TWOPI=2.0*PI
C
C      ENTER HOLE-FORMATION GEOMETRY, AND FORMATION FLOW PARAMETERS
C
100  WRITE (*,10000)
      READ (*,15000,ERR=100) OUTPUT
      OPEN (2,FILE=OUTPUT,STATUS='NEW')
200  WRITE (*,20000)
      READ (*,*,ERR=200) VIS,PAVG
300  WRITE (*,25000)
      READ (*,*,ERR=300) RMIN,RMAX
350  WRITE (*,26000)
      READ (*,*,ERR=350) NCHIM
400  WRITE (*,30000)
      READ (*,*,ERR=400) NLAYER
          DO 800 N=1,NLAYER
500      WRITE (*,35000) N
          WRITE (*,40000)
          READ (*,*,ERR=500) PERM(N),POR(N),THICKL(N)
          PERM(N)=9.86923E-13*PERM(N)
550      WRITE (*,41000)
          READ (*,*,ERR=550) PERM2(N),POR2(N)
          PERM2(N)=9.86923E-13*PERM2(N)
600      WRITE (*,45000)
          READ (*,*,ERR=600) NV(N)
          IF (NV(N).LT.2) GO TO 600
800      CONTINUE

```

```

C
C      COMPUTE NODAL COORDINATES
C      WRITE(*,74000)
C
C
C      DR=RMIN/(NCHIM-1)
C
C      SET RADIAL COORDINATES FOR CHIMNEY
C      DO 850 I=1,NCHIM
C      RC(I)=FLOAT(I-1)*DR
850  CONTINUE
C      I=NCHIM
C
C      SET RADIAL COORDINATES FOR FORMATION
C      900  I=I+1
C      RC(I)=DR*2.0** (I-1-NCHIM)+RMIN
C      IF (RC(I)-RMAX) 900,1000,1000
1000  RC(I)=RMAX
C      NC=I
C      IF (NC.GT.20) GOTO 71000
C      D=0
C      ZC(1)=0
C      NR=1
C      DO 1200 I=1,NLAYER
C      DD=THICKL(I)/NV(I)
C      DO 1100 J=1,NV(I)
C      D=D+DD
C      NR=NR+1
1100  ZC(NR)=D
1200  NV(I)=NR
C
C      IF (NR.GT.200) GOTO 73000
C
C      COMPUTE NODAL CONDUCTIVITIES AND STORAGE FACTORS
C
C      L=1
C      DO 1400 J=1,NR
C      IF (J.GT.NV(L)) L=L+1
C      DZ=ZC(MIN0(J+1,NR))-ZC(MAX0(J-1,1))
C      DO 1300 I=1,NC
C      IF (I.GT.NCHIM) GOTO 1250
C      CL=PERM2(L)/VIS
C      SFL=PDR2(L)/PAVG
C      GOTO 1260
1250  CL=PERM(L)/VIS
C      SFL=PDR(L)/PAVG
1260  DR=RC(MIN0(I+1,NC))-RC(MAX0(I-1,1))
C      IF (I.NE.NC) C(I,J,2)=CL*DZ/((RC(I+1)-RC(I))*2.0)
C      IF (J.NE.NR) C(I,J,1)=CL*DR/((ZC(J+1)-ZC(J))*2.0)
C      SF(I,J)=SFL*DZ*DR/4.0
C      P(I,J)=PAVG
1300  Q(I,J)=0.0
C
C      SET BOUNDARY NODES
C
C

```

```

1400      C(NC,J,2)=0.0
C
C      SET NO-FLOW CONDITION AT BOTTOM BOUNDARY
DO 1500 I=1,NC
1500      C(I,NR,1)=0.0
C
C      REFINE NODAL VALUES ON BOUNDARIES OF HORIZONTAL LAYERS
C
      IF (NLAYER.EQ.1) GO TO 1700
      DO 1600 L=1,NLAYER-1
      DO 1600 I=1,NC
      C(I,NV(L),1)=C(I,NV(L)+1,1)
      C(I,NV(L),2)=(C(I,NV(L)-1,2)+C(I,NV(L)+1,2))/2.0
1600      SF(I,NV(L))=(SF(I,NV(L)-1)+SF(I,NV(L)+1))/2.0
C
C      CONVERT FOR RADIAL FLOW WIDTHS
C
1700      DO 1900 J=1,NR
      DO 1800 I=2,NC-1
      C(I,J,1)=C(I,J,1)*(RC(I-1)+RC(I+1))*PI
      SF(I,J)=SF(I,J)*(RC(I-1)+RC(I+1))*PI
1800      C(I,J,2)=C(I,J,2)*(RC(I)+RC(I+1))*PI
      C(NC,J,1)=C(NC,J,1)*(RC(NC-1)+0.75*(RC(NC)-RC(NC-1)))*TWOPI
      SF(NC,J)=SF(NC,J)*(RC(NC-1)+0.75*(RC(NC)-RC(NC-1)))*TWOPI
      SF(1,J)=SF(1,J)*RC(2)*PI/2.0
      C(1,J,1)=C(1,J,1)*0.25*RC(2)*PI
1900      C(1,J,2)=C(1,J,2)*0.50*RC(2)*PI
C
C      WRITE INPUT FILE
C
      WRITE (2,55000) VIS,PAVG,NLAYER,NC,NR,NCHIM
      WRITE (2,60000) (RC(I),I=1,NC)
      WRITE (2,60000) (ZC(I),I=1,NR)
      WRITE (2,65000) (NV(I),PERM(I),POR(I),I=1,NLAYER)
      WRITE (2,65000) (NV(I),PERM2(I),POR2(I),I=1,NLAYER)
      DO 2000 J=1,NR
      DO 2000 I=1,NC
      WRITE (2,60000) C(I,J,1),C(I,J,2),SF(I,J),P(I,J),Q(I,J)
2000      CONTINUE
      GOTO 75000
      CLOSE (2)
10000 FORMAT(' ENTER GENERAL OUTPUT FILE NAME: ',%)
15000 FORMAT(A)
20000 FORMAT(/,' ENTER FLUID VISCOSITY (Pa-sec) AND',
X' MEAN PRESSURE (Pa): ',%)
25000 FORMAT(/,' ENTER CHIMNEY RADIUS (m) AND OUTER RADIUS (m): ',%)
26000 FORMAT(/,' ENTER NO. RADIAL NODES IN CHIMNEY ',%)
30000 FORMAT(/,' ENTER NUMBER OF LAYERS: ',%)
35000 FORMAT(///,' FOR LAYER NUMBER:',I3)
40000 FORMAT(/,' ENTER FORMATION PERMEABILITY (d), POROSITY, AND'
X' THICKNESS (m): ',%)
41000 FORMAT(/,' ENTER CHIMNEY PERMEABILITY (d) AND POROSITY ',%)
45000 FORMAT(/,' ENTER NUMBER OF VERTICAL NODES IN LAYER',
X' MINIMUM OF 2: ',%)
55000 FORMAT(2E15.6,4I15)

```



```
60000 FORMAT(5E15.6)
65000 FORMAT(I15,2E15.6)
70000 FORMAT(' OOPS..NEED MORE THAN 20 RADIAL NODES',/,
X ' CHANGE DIMENSION STATEMENTS OF CHAN AND RCHAN')
71000 WRITE(*,70000)
      GOTO 75000
72000 FORMAT(' OOPS..NEED MORE THAN 200 VERTICAL NODES',/,
X ' CHANGE DIMENSION STATEMENTS OF CHAN AND RCHAN',/,
X ' OR REDUCE NO. NODES ASSIGNED TO LAYERS')
73000 WRITE(*,72000)
74000 FORMAT(/,' WRITING FINITE DIFFERENCE MESH DATA FILE')
75000 STOP
      END
```

```

C      ++++++
C      +//
C      +// CHAN (CHimney Analysis) //
C      +//
C      ++++++
C
C      WRITTEN BY:
C      JONATHAN M. HANSON
C      HANSON & ASSOCIATES
C      SALT LAKE CITY, UT 84108
C      AUGUST, 1985
C
C      APPLICATION:
C      CHAN CALCULATES THE PRESSURE RESPONSE AT A POINT WITHIN A
C      NUCLEAR CHIMNEY OR AWAY FROM THE CHIMNEY DUE TO A SURFACE
C      BAROMETRIC PRESSURE VARIATION. AN ITERATED ALTERNATING
C      DIRECTION IMPLICIT FINITE DIFFERENCE METHOD IS USED IN THE
C      CALCULATION.
C
C      BASED ON:
C      PRICKETT, T.A. AND C.G. LONNQUIST
C      SELECTED DIGITAL COMPUTER TECHNIQUES FOR GROUNDWATER
C      RESOURCE EVALUATION
C      ILLINOIS STATE WATER SURVEY, URBANA, BULLETIN 55, 1971
C
C      DEFINITION OF VARIABLES
C
C      NSTEPS - NUMBER OF TIME STEPS
C      DELTA  - SIZE OF TIME STEP (Secs)
C      ERROR  - MAXIMUM ALLOWED CONVERGENCE ERROR (Pa)
C      NC     - NUMBER OF NODAL COLUMNS
C      NR     - NUMBER OF NODAL ROWS
C      P(I,J) - NODAL PRESSURE AT CURRENT TIME STEP (Pa)
C      PO(I,J) - NODAL PRESSURE AT PREVIOUS TIME STEP (Pa)
C      DL(I,J) - CHANGE IN PRESSURE FROM PREVIOUS TIME STEP (Pa)
C      SF(I,J) - STORAGE COEFFICIENT (POROSITY * NODAL AREA / MEAN
C               ABSOLUTE PRESSURE) (sq.m./Pa)
C      Q(I,J) - TRUE VOLUMETRIC FLUX PER UNIT THICKNESS (cu.m./sec)
C      QT     - TOTAL VOLUME INFLUX INTO WELL (cu.m)
C      C(I,J,1) - NODAL CONDUCTIVITY IN Y-DIRECTION (sq. meter/Pa-sec)
C      C(I,J,2) - NODAL CONDUCTIVITY IN X-DIRECTION
C      PAVG    - AVERAGE ATMOSPHERIC PRESSURE (Pa)
C      VIS     - VISCOSITY OF FLUID (Pa-sec)
C      PERM(I) - PERMEABILITY OF LAYER I (sq.m.)
C      POR(I)  - POROSITY OF LAYER I
C
C      $DEBUG
C      $NOFLOATCALLS
C      $LARGE
C
C      DIMENSION P(20,200), PO(20,200), SF(20,200),
X      C(20,200,2), DL(20,200), RC(20), ZC(200), Q(20,200),
X      NV(10), PERM(10), POR(10), PERM2(10), POR2(10)
C      DOUBLE PRECISION B(200), G(200), W, AA, BB, CC, DD
C      CHARACTER*20 INPUT, OUTPUT, PINPUT, FNAME, RNAME

```

```

C
C
C   READ INPUT PARAMETERS
C
  WRITE (*,10000)
  READ (*,16000) INPUT
  OPEN (1,FILE=INPUT,STATUS='OLD')
  WRITE (*,18000)
  READ (*,16000) OUTPUT
  OPEN (2,FILE=OUTPUT,STATUS='NEW')
  WRITE (*,20000)
  READ (*,*) NSTEPS,IOUT
  WRITE (*,22000)
  READ (*,*) DELTA,ERROR
C
C   CHANGE DELTA TO SECONDS
  DELTA=DELTA*3600.
C
  WRITE (*,24000)
  READ (*,*) MODE
C
C
C   SET UP PRESSURE VS TIME OUTPUT FILE
  WRITE (*,50000)
  READ (*,16000) FNAME
  OPEN (3,FILE=FNAME,STATUS='NEW')
C
C   INITIALIZE PRESSURE VS DEPTH (OUTER BOUNDARY) FILE
  WRITE(*,55000)
  READ(*,16000) RNAME
  OPEN (7,FILE=RNAME, STATUS='NEW')
C
C
C   READ INFORMATION FROM DISK FILE (GENERATED BY RCHAN)
  READ (1,26000) VIS,PAVG,NLAYER,NC,NR
  READ (1,28000) (RC(I),I=1,NC)
  READ (1,28000) (ZC(I),I=1,NR)
  READ (1,30000) (NV(I),PERM(I),POR(I),I=1,NLAYER)
  READ (1,30000) (NV(I),PERM2(I),POR2(I),I=1,NLAYER)
C
  WRITE(*,10500) NC,NR
C
C   READ NODE NUMBER FOR OUTPUT PRESSURE VS TIME FILE
  WRITE(*,11000)
  READ(*,*) IRAD,IDEP
C
C   WRITE LOCATION OF SENSOR
  WRITE(*,11500) RC(IRAD),ZC(IDEP)
C
C   SET CONSTANT PRESSURE BOUNDARY (SURFACE)
C
100 WRITE (*,32000)
   READ (*,*,ERR=100) NTC
   IF (NTC.EQ.2) GO TO 300
200 WRITE (*,34000)

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      READ (*,*,ERR=200) PUPPER
      GO TO 400
C
300 WRITE (*,10000)
      READ (*,16000,ERR=300) PINPUT
      OPEN (6,FILE=PINPUT,STATUS='OLD')
C
      READ NODE CARDS
C
400 WRITE (*,12000)
      DO 600 J=1,NR
          DO 600 I=1,NC
              READ (1,28000) C(I,J,1),C(I,J,2),SF(I,J),P(I,J),Q(I,J)
              IF (MODE.EQ.1) P(I,J)=P(I,J)-PAVG
              PO(I,J)=P(I,J)
          600 CONTINUE
C
      REWIND(1)
      CLOSE(1)
C
      SET UPPER BOUNDARY
      IF (NTC.EQ.2) GO TO 900
700   DO 800 I=1,NC
          SF(I,1)=1.0E25
          P(I,1)=PUPPER
      800   PO(I,1)=PUPPER
      GO TO 1100
900   DO 1000 I=2,NC
1000   SF(I,1)=1.E25
      READ (6,56000) PUPPER,ETIME
      GO TO 700
C
      PRINT INPUT PARAMETERS
C
1100 WRITE (2,36000) DELTA,ERROR,VIS,PAVG
      WRITE (2,38000)
      WRITE (2,40000) (I,PERM(I),POR(I),I=1,NLAYER)
      WRITE (2,40000) (I,PERM2(I),POR2(I),I=1,NLAYER)
      WRITE (2,42000)
      WRITE (2,44000) (I,RC(I),I=1,NC)
      WRITE (2,46000)
      L=1
          DO 1200 J=1,NR
              IF (J.GT.NV(L)) L=L+1
              WRITE (2,48000) J,L,ZC(J)
1200 CONTINUE
C
      INITIALIZE OUTPUT DATA FILES
      WRITE (3,*) NSTEPS
      WRITE (7,*) NR
C
      START OF SIMULATION
C

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```

WRITE (*,14000)
1300 TIME=0.0
   QT=0.0
      DO 4500 ISTEP=1,NSTEPS
         TIME=TIME+DELTA
C
C      READ UPPER BOUNDARY PRESSURES IF TIME VARYING
C
      IF (NTC.EQ.1) GO TO 1500
      IF (TIME.LT.ETIME) GO TO 1500
      READ (6,56000) PUPPER,ETIME
      DO 1400 I=2,NC
1400    P(I,1)=PUPPER
C
C      PREDICT PRESSURES FOR NEXT TIME INCREMENT
C
1500    DO 1700 I=1,NC
      DO 1700 J=1,NR
      IF (SF(I,J).GT.1.0E20) P(I,J)=PO(I,J)
      D=P(I,J)-PO(I,J)
      PO(I,J)=P(I,J)
      F=1.0
      P(I,J)=P(I,J)+D*F
1700
C
C      REFINE ESTIMATES OF PRESSURES BY IADI METHOD
C
      ITER=0
      E=0.0
1800    ITER=ITER+1
C
C      COLUMN CALCULATIONS
C
      DO 3000 II=1,NC
      I=II
      IF (MOD(ISTEP+ITER,2).EQ.1) I=NC-I+1
      DO 2800 J=1,NR
C
C      CALCULATE B AND G ARRAYS
C
      BB=SF(I,J)/DELTA
      DD=PO(I,J)*SF(I,J)/DELTA+Q(I,J)
      IF (J-1) 1900,2000,1900
1900    AA=-C(I,J-1,1)
      BB=BB+C(I,J-1,1)
2000    IF (J-NR) 2100,2200,2100
2100    CC=-C(I,J,1)
      BB=BB+C(I,J,1)
2200    IF (I-1) 2300,2400,2300
2300    BB=BB+C(I-1,J,2)
      DD=DD+P(I-1,J)*C(I-1,J,2)
2400    IF (I-NC) 2500,2600,2500
2500    BB=BB+C(I,J,2)
      DD=DD+P(I+1,J)*C(I,J,2)
2600    W=BB

```

```

                IF (J-1) 2700, 2700, 2650
2650            W=BB-AA*B(J-1)
2700            B(J)=CC/W
                G(J)=DD/W
                IF (J-1) 2800, 2800, 2750
2750            G(J)=G(J)-AA*B(J-1)/W
2800            CONTINUE
C
C            RE-ESTIMATE PRESSURES
C
                EN=ABS(P(I, NR)-G(NR))
                E=AMAX1(E, EN)
                P(I, NR)=G(NR)
                N=NR-1
2900            HA=G(N)-B(N)*P(I, N+1)
                EN=ABS(HA-P(I, N))
                E=AMAX1(E, EN)
                P(I, N)=HA
                N=N-1
                IF (N) 3000, 3000, 2900
3000            CONTINUE
C
C            ROW CALCULATIONS
C
                DO 4100 JJ=1, NR
                J=JJ
                IF (MOD(ISTEP+ITER, 2).EQ.1) J=NR-J+1
                DO 3900 I=1, NC
                BB=SF(I, J)/DELTA
                DD=PO(I, J)*SF(I, J)/DELTA+Q(I, J)
                IF (J-1) 3100, 3200, 3100
3100            BB=BB+C(I, J-1, 1)
                DD=DD+P(I, J-1)*C(I, J-1, 1)
3200            IF (J-NR) 3300, 3400, 3300
3300            DD=DD+P(I, J+1)*C(I, J, 1)
                BB=BB+C(I, J, 1)
3400            IF (I-1) 3500, 3600, 3500
3500            BB=BB+C(I-1, J, 2)
                AA=-C(I-1, J, 2)
3600            IF (I-NC) 3700, 3800, 3700
3700            BB=BB+C(I, J, 2)
                CC=-C(I, J, 2)
3800            W=BB
                IF (I-1) 3850, 3850, 3840
3840            W=W-AA*B(I-1)
3850            B(I)=CC/W
                G(I)=DD/W
                IF (I-1) 3900, 3900, 3860
3860            G(I)=G(I)-AA*G(I-1)/W
3900            CONTINUE
C
C            RE-ESTIMATE PRESSURES
C
                EN=ABS(P(NC, J)-G(NC))
                E=AMAX1(E, EN)

```

```

        P(NC,J)=G(NC)
        N=NC-1
4000    HA=G(N)-B(N)*P(N+1,J)
        EN=ABS(P(N,J)-HA)
        E=AMAX1(E,EN)
        P(N,J)=HA
        N=N-1
        IF (N) 4100,4100,4000
4100    CONTINUE
        WRITE(*,50000) ISTEP,ITER,E

        IF (E.GT.ERROR) GO TO 1800

C
C
C
C    WRITE CALCULATED PRESSURE ONTO FILE
        TIM2=TIME/3600.
        PZAPT=P(IRAD,IDEF)
        IF(MODE.EQ.0) PZAPT=PZAPT-PAVG
        WRITE(3,*) TIM2,PZAPT
        WRITE(*,60000) TIM2,PZAPT

C
C
C
C    PRINT RESULTS

        IF (IOUT*(ISTEP/IOUT).NE.ISTEP) GO TO 4500

C
C    WRITE CURRENT RESULTS ON OUTPUT FILES
        KOUNT=(NC-1)/6+1
        DO 4400 K=1,KOUNT
            I1=1+(K-1)*6
            I2=K*6
            IF (I2.GT.NC) I2=NC
            WRITE(2,62000) TIME,PAVG,QT
            WRITE(2,64000) (I,I=I1,I2)
            DO 4400 J=1,NR
                WRITE(2,66000) J,(P(I,J),I=I1,I2)
4400        CONTINUE
4500    CONTINUE

C
C
C    WRITE P(Z) AND DP/DR (Z) ONTO FILES
        DO 4600 J=1,NR
            PZAPIN=P(1,J)
            PZAPOUT=P(NC,J)
            IF(MODE.EQ.0) PZAPIN=PZAPIN-PAVG
            IF(MODE.EQ.0) PZAPOUT=PZAPOUT-PAVG

C
            WRITE(7,*) ZC(J),PZAPOUT
4600    CONTINUE

C
        CLOSE(2)
        CLOSE(3)
        CLOSE(6)
        CLOSE(7)

```

```

STOP
10000 FORMAT(/, ' ENTER INPUT FILE NAME: ', $)
10500 FORMAT(/, ' NODAL MESH HAS ', I3, ' COLUMNS (RADIAL COORDINATE)', /,
X      ' AND ', I3, ' ROWS (DEPTH COORDINATE) ')
11000 FORMAT(/, ' ENTER RADIAL AND VERTICAL NODE OF SENSOR ', $)
11500 FORMAT(/, ' SENSOR IS LOCATED AT:', /,
X      ' R = ', E12.4, ' m', /,
X      ' Z = ', E12.4, ' m', /)
12000 FORMAT(/, ' READING FINITE DIFFERENCE MESH DATA FILE', /)
14000 FORMAT(/, ' BEGIN SIMULATION', /,
X      ' ITERATED ALTERNATING DIRECTION IMPLICIT (IADI)', /,
X      ' FINITE DIFFERENCE METHOD', /)
15000 FORMAT(A)
18000 FORMAT(/, ' ENTER OUTPUT FILE NAME: ', $)
20000 FORMAT(/, ' ENTER TOTAL NUMBER OF TIME STEPS AND THE ', /,
X      ' NUMBER OF TIME STEPS BETWEEN LISTINGS: ', $)
22000 FORMAT(/, ' ENTER SIZE OF TIME STEP (HRS) AND THE ', /,
X      ' MAXIMUM PRESSURE CHANGE PER NODE (Pa)', /,
X      ' TO CONVERGENCE: ', $)
24000 FORMAT(/, ' ABSOLUTE (0) OR GAGE (1) PRESSURE COMPUTATION? ', $)
25000 FORMAT(2E15.6, 3I15)
28000 FORMAT(5E15.6)
30000 FORMAT(I15, 2E15.6)
32000 FORMAT(/, ' CONSTANT (1) OR TIME VARYING (2) SURFACE PRESSURE ', $)
34000 FORMAT(/, ' ENTER UPPER BOUNDARY PRESSURE (Pa): ', $)
36000 FORMAT('1', //, ' PSEUDO 3D BAROMETRIC GAS FLOW MODEL', //,
X      ' THE INPUT PARAMETERS FOR THIS RUN ARE:', //, ' TIME STEP:',
XT30, E16.4, ' Sec', /, ' ERROR LIMIT:', T30, E16.4, ' Pa', /,
X      ' VISCOSITY:', T30, E16.4, ' Pa-sec', /,
X      ' MEAN BAROMETRIC PRESSURE:', T30, E16.4, ' Pa')
38000 FORMAT(/, T5, ' LAYER NO.', T20, ' PERMEABILITY (sq.m.)', T45,
X      ' POROSITY', /)
40000 FORMAT(T5, I5, T20, E14.3, T45, E9.3)
42000 FORMAT(/, ' RADIAL COORDINATES', //, T5, ' NODE NO.',
XT20, ' DISTANCE (m)')
44000 FORMAT(T5, I5, T20, F10.2)
46000 FORMAT(/, ' VERTICAL COORDINATES', //, T5, ' NODE NO.',
XT20, ' LAYER NO.', T35, ' DISTANCE (m)')
48000 FORMAT(T5, I5, T20, I5, T35, F10.2)
50000 FORMAT(/, ' PRESSURE VS TIME OUTPUT FILE NAME? ', $)
55000 FORMAT(/, ' PRESSURE VS DEPTH (OUTER BOUNDARY) OUTPUT FILENAME? ',
X      $)
56000 FORMAT(2E15.4)
58000 FORMAT(' ISTEP=', I4, ' ITER=', I4, ' MAX DELTA P=',
XE12.4)
60000 FORMAT(/, ' TIME (Hrs) =', E12.4, /,
X      ' SENSOR PRESSURE (Pa) =', E12.4, /)
62000 FORMAT('1 NODAL PRESSURES (Pa)', //, T5, ' TIME= ',
XF10.0, ' secs', /, T5, ' PAVG= ', E15.4, ' Pascals', /, T5,
X      ' TOTAL VOLUME FLUX INTO WELL= ', E15.4, ' cu.m.')
64000 FORMAT(' J=\\I= ', 6(I2, 10X))
66000 FORMAT(/, I4, I3, 6E12.5)
END

```



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C      ++++++
C      +//////////
C      +////////// FCHAN (Frequency domain CHimney ANalysis) //////////
C      +//////////
C      ++++++
C
C      WRITTEN BY:
C      JONATHAN M. HANSON
C      HANSON & ASSOCIATES
C      SALT LAKE CITY, UT 84108
C      AUGUST, 1985
C
C      APPLICATION:
C      FCHAN CALCULATES THE PRESSURE RESPONSE AT A POINT WITHIN A
C      NUCLEAR CHIMNEY OR AWAY FROM THE CHIMNEY DUE TO A SURFACE
C      BAROMETRIC PRESSURE VARIATION. CALCULATIONS ARE CARRIED OUT
C      IN THE FREQUENCY DOMAIN, GIVEN A SURFACE PRESSURE SIGNAL OF
C      THE FORM  $P=P0*EXP(IWT)$ , WHERE W IS ANGULAR FREQUENCY.
C      AN ITERATED ALTERNATING DIRECTION IMPLICIT FINITE DIFFERENCE
C      METHOD IS USED IN THE CALCULATION.
C
C      BASED ON:
C      PRICKETT, T.A. AND C.G. LONNQUIST
C      SELECTED DIGITAL COMPUTER TECHNIQUES FOR GROUNDWATER
C      RESOURCE EVALUATION
C      ILLINOIS STATE WATER SURVEY, URBANA, BULLETIN 55, 1971
C
C      DEFINITION OF VARIABLES
C
C      NSTEPS - NUMBER OF TIME STEPS
C      DELTA - SIZE OF TIME STEP (Secs)
C      ERROR - MAXIMUM ALLOWED CONVERGENCE ERROR (Pa)
C      NC - NUMBER OF NODAL COLUMNS
C      NR - NUMBER OF NODAL ROWS
C      P(I,J) - NODAL PRESSURE AT CURRENT TIME STEP (Pa)
C      P0(I,J) - NODAL PRESSURE AT PREVIOUS TIME STEP (Pa)
C      DL(I,J) - CHANGE IN PRESSURE FROM PREVIOUS TIME STEP (Pa)
C      SF(I,J) - STORAGE COEFFICIENT (POROSITY * NODAL AREA / MEAN
C      ABSOLUTE PRESSURE) (sq.m./Pa)
C      Q(I,J) - TRUE VOLUMETRIC FLUX PER UNIT THICKNESS (cu.m./sec)
C      QT - TOTAL VOLUME INFLUX INTO WELL (cu.m)
C      C(I,J,1) - NODAL CONDUCTIVITY IN Y-DIRECTION (sq. meter/Pa-sec)
C      C(I,J,2) - NODAL CONDUCTIVITY IN X-DIRECTION
C      PAVG - AVERAGE ATMOSPHERIC PRESSURE (Pa)
C      VIS - VISCOSITY OF FLUID (Pa-sec)
C      PERM(I) - FORMATION PERMEABILITY OF LAYER I (sq.m.)
C      POR(I) - FORMATION POROSITY OF LAYER I
C      PERM2(I) - CHIMNEY PERMEABILITY OF LAYER I (sq. m.)
C      POR2(I) - CHIMNEY POROSITY OF LAYER I
C
C      $DEBUG
C      $NOFLOATCALLS
C      $LARGE
C      DIMENSION SF(20,200),
C      X C(20,200,2), DL(20,200), RC(20), ZC(200), Q(20,200),

```

```

X  NV(10),PERM(10),POR(10),PERM2(10), POR2(10)
   COMPLEX D,F,HA,B(200),G(200),W,AA,BB,CC,DD,PZAPIN,PZAPOUT
   COMPLEX DELP,ARG2
   COMPLEX P(20,200),PG(20,200)
   CHARACTER*20 INPUT,OUTPUT,PINPUT,FNAME,RNAME

C
   TWOPI=6.283185308

C
C   READ INPUT PARAMETERS
C
   WRITE (*,10000)
   READ (*,16000) INPUT
   OPEN (1,FILE=INPUT,STATUS='OLD')
   WRITE (*,18000)
   READ (*,16000) OUTPUT
   OPEN (2,FILE=OUTPUT,STATUS='NEW')
   WRITE (*,20000)
   READ (*,*) NSTEPS, IOUT
   WRITE (*,22000)
   READ (*,*) FMIN,FMAX,ERROR

C
C
C   SET UP PRESSURE VS FREQUENCY OUTPUT FILE
   WRITE (*,50000)
   READ (*,16000) FNAME
   OPEN (3,FILE=FNAME,STATUS='NEW')

C
C   INITIALIZE PRESSURE VS DEPTH (OUTER BOUNDARY) FILE
   WRITE (*,55000)
   READ (*,16000) RNAME
   OPEN (7,FILE=RNAME, STATUS='NEW')

C
C
C   READ INFORMATION FROM DISK FILE (GENERATED BY RUNBFD)
C
   READ (1,26000) VIS,PAVG,NLAYER,NC,NR,NCHIM
   READ (1,28000) (RC(I),I=1,NC)
   READ (1,28000) (ZC(I),I=1,NR)
   READ (1,30000) (NV(I),PERM(I),POR(I),I=1,NLAYER)
   READ (1,30000) (NV(I),PERM2(I),POR2(I),I=1,NLAYER)

C
   WRITE(*,10500) NC,NR

C
C   READ NODE NUMBER FOR OUTPUT PRESSURE VS FREQUENCY FILE
   WRITE(*,11000)
   READ(*,*) IRAD, IDEP

C
C   WRITE LOCATION OF SENSOR
   WRITE(*,11500) RC(IRAD),ZC(IDEP)

C
C   SET CONSTANT PRESSURE BOUNDARY (SURFACE)
C
200 WRITE (*,34000)
   READ (*,*,ERR=200) PUPPER

```

```

C
C   READ NODE CARDS
C
400 WRITE (*,12000)
      DO 600 J=1,NR
        DO 600 I=1,NC
          READ (1,28000) C(I,J,1),C(I,J,2),SF(I,J),PP,Q(I,J)
600      CONTINUE
C
      REWIND(1)
      CLOSE(1)
C
C   SET UPPER BOUNDARY
700   DO 800 I=1,NC
800   SF(I,1)=1.1E10
C
C   PRINT INPUT PARAMETERS
C
1100 WRITE (2,36000) DELTA,ERROR,VIS,PAVG
      WRITE (2,38000)
      WRITE (2,40000) (I,PERM(I),POR(I),I=1,NLAYER)
      WRITE (2,40000) (I,PERM2(I),POR2(I),I=1,NLAYER)
      WRITE (2,42000)
      WRITE (2,44000) (I,RC(I),I=1,NC)
      WRITE (2,46000)
      L=1
      DO 1200 J=1,NR
        IF (J.GT.NV(L)) L=L+1
        WRITE (2,48000) J,L,ZC(J)
1200    CONTINUE
C
C
C   INITIALIZE OUTPUT DATA FILES
      WRITE (3,*) NSTEPS
      WRITE (7,*) NR
C
C
C   START OF SIMULATION
C
      WRITE (*,14000)
1300 OMIN=TWOPI*FMIN/3600.
      OMAX=TWOPI*FMAX/3600.
C
C   NOTE: COMPUTATIONS IN FREQUENCY SPACE REQUIRE FREQ. IN
C         RADIANS/SEC. - HENCE, THE DIVISION BY 3600.
      DOMEGA=(OMAX-OMIN)/FLOAT(NSTEPS-1)
C
C   INITIALIZE PRESSURE DISTRIBUTION USING HOMOGENEOUS AND ISOTROPIC
C   HALF-SPACE MODEL.
      WRITE(*,*) ' BEGIN INITIALIZATION OF NODE MESH'
      L=1
      DO 1350 J=1,NR
        IF(J.GT.NV(L)) L=L+1
      DO 1350 I=1,NC
        IF(I.GT.NCHIM) DIFF=PERM(L)*PAVG/(VIS*POR(L))

```

```

      IF (I.LE.NCHIM) DIFF=PERM2(L)*PAVG/(VIS*POR2(L))
      P(I,J)=PUPPER*CEXP(-CMPLX(0.70710678,0.70710678)
X      *SQRT(OMIN/DIFF)*ZC(J))
1350 PO(I,J)=P(I,J)
      WRITE(*,*) ' NODE MESH INITIALIZATION COMPLETE'
C
      DO 4500 ISTEP=1,NSTEPS
      OMEGA=OMIN+FLOAT(ISTEP-1)*DOMEGA
      IF(ISTEP.EQ.1) GOTO 1750
C
C      PREDICT PRESSURES FOR NEXT FREQUENCY INCREMENT
C
      WRITE(*,*) ' PREDICT PRESSURE FOR STEP', ISTEP
      L=1
1500. DO 1700 J=1,NR
      IF(J.GT.NV(L)) L=L+1
      DO 1700 I=1,NC
      IF (SF(I,J).GT.1.0E10) P(I,J)=PO(I,J)
      PO(I,J)=P(I,J)
      IF(J.EQ.1) GOTO 1700
      IF (I.GT.NCHIM) DIFF=PERM(L)*PAVG/(VIS*POR(L))
      IF (I.LE.NCHIM) DIFF=PERM2(L)*PAVG/(VIS*POR2(L))
      ARG=SQRT(OMEGA/(2.0*DIFF))
      ARG2=CMPLX(0.0,ZC(J)/(2.0*DIFF))
      DELP=-PO(I,J)*DOMEGA*ARG2/
X      CMPLX(ARG,ARG)
      P(I,J)=P(I,J)+DELP
1700 CONTINUE
C
C      REFINE ESTIMATES OF PRESSURES BY IADI METHOD
C
1750 ITER=0
1800 E=0.0
      ITER=ITER+1
C
C      COLUMN CALCULATIONS
C
      DO 3000 II=1,NC
      I=II
      IF (MOD(ISTEP+ITER,2).EQ.1) I=NC-I+1
      DO 2800 J=1,NR
C
C      CALCULATE B AND G ARRAYS
C
      BB=CMPLX(0.0,OMEGA*SF(I,J))
      DD=CMPLX(0.0,0.0)
      IF(J.EQ.1) DD=CMPLX(0.0,OMEGA*SF(I,J))*P(I,J)
      IF (J-1) 1900,2000,1900
1900 AA=CMPLX(-C(I,J-1,1),0.0)
      BB=BB+CMPLX(C(I,J-1,1),0.0)
2000 IF (J-NR) 2100,2200,2100
2100 CC=CMPLX(-C(I,J,1),0.0)
      BB=BB+CMPLX(C(I,J,1),0.0)
2200 IF (I-1) 2300,2400,2300

```

```

2300      BB=BB+CMPLX(C(I-1,J,2),0.0)
          DD=DD+P(I-1,J)*CMPLX(C(I-1,J,2),0.0)
2400      IF (I-NC) 2500,2500,2500
2500      BB=BB+CMPLX(C(I,J,2),0.0)
          DD=DD+P(I+1,J)*CMPLX(C(I,J,2),0.0)
2600      W=BB
          IF (J-1) 2700,2700,2650
2650      W=BB-AA*B(J-1)
2700      B(J)=CC/W
          G(J)=DD/W
          IF (J-1) 2800,2800,2750
          G(J)=G(J)-AA*G(J-1)/W
2750
2800      CONTINUE

```

```

C
C      RE-ESTIMATE PRESSURES
C

```

```

          EN=CABS(P(I,NR)-G(NR))
          E=AMAX1(E,EN)
          P(I,NR)=G(NR)
          N=NR-1
2900      HA=G(N)-B(N)*P(I,N+1)
          EN=CABS(HA-P(I,N))
          E=AMAX1(E,EN)
          P(I,N)=HA
          N=N-1
          IF (N) 3000,3000,2900
3000      CONTINUE

```

```

C
C      ROW CALCULATIONS
C

```

```

          DO 4100 JJ=1,NR
          J=JJ
          IF (MOD(ISTEP+ITER,2).EQ.1) J=NR-J+1
          DO 3900 I=1,NC
          BB=CMPLX(0.0,OMEGA*SF(I,J))
          DD=CMPLX(0.0,0.0)
          IF (J.EQ.1) DD=CMPLX(0.0,OMEGA*SF(I,J))*P(I,J)
          IF (J-1) 3100,3200,3100
          BB=BB+CMPLX(C(I,J-1,1),0.0)
          DD=DD+P(I,J-1)*CMPLX(C(I,J-1,1),0.0)
          IF (J-NR) 3300,3400,3300
          DD=DD+P(I,J+1)*CMPLX(C(I,J,1),0.0)
          BB=BB+CMPLX(C(I,J,1),0.0)
          IF (I-1) 3500,3600,3500
          BB=BB+CMPLX(C(I-1,J,2),0.0)
          AA=CMPLX(-C(I-1,J,2),0.0)
          IF (I-NC) 3700,3800,3700
          BB=BB+CMPLX(C(I,J,2),0.0)
          CC=CMPLX(-C(I,J,2),0.0)
          W=BB
          IF (I-1) 3850,3850,3840
          W=W-AA*B(I-1)
          B(I)=CC/W
          G(I)=DD/W
          IF (I-1) 3900,3900,3860

```

```

3850          G(I)=G(I)-AA*G(I-1)/W
3900          CONTINUE
C
C          RE-ESTIMATE PRESSURES
C
          EN=CABS(P(NC,J)-G(NC))
          E=AMAX1(E,EN)
          P(NC,J)=G(NC)
          N=NC-1
4000          HA=G(N)-B(N)*P(N+1,J)
          EN=CABS(P(N,J)-HA)
          E=AMAX1(E,EN)
          P(N,J)=HA
          N=N-1
          IF (N) 4100,4100,4000
4100          CONTINUE
          WRITE (*,58000) ISTEP,ITER,E
          IF (E.GT.ERROR) GO TO 1800
C
          DO 4105 J=1,NR
4105          CONTINUE
C
C
C          WRITE CALCULATED PRESSURE ONTO FILE
          FREQ=OMEGA*3600./TWOPI
          PREAL=REAL(P(IRAD,IDEF))
          PIMAG=AIMAG(P(IRAD,IDEF))
          AMP=SQRT(PREAL*PREAL+PIMAG*PIMAG)
          PHASE=(360./TWOPI)*ATAN2(PIMAG,PREAL)
          WRITE (3,59000) FREQ,PREAL,PIMAG,AMP,PHASE
          WRITE (*,60000) FREQ,PREAL,PIMAG,AMP,PHASE
C
C
C          PRINT RESULTS
C
          IF (IOUT*(ISTEP/IOUT).NE.ISTEP) GO TO 4500
C
C          WRITE CURRENT RESULTS ON OUTPUT FILES
          KOUNT=(NC-1)/5+1
          DO 4400 K=1,KOUNT
          I1=1+(K-1)*6
          I2=K*6
          IF (I2.GT.NC) I2=NC
          WRITE (2,64000) (I,I=I1,I2)
          DO 4400 J=1,NR
          WRITE (2,66000) J,(P(I,J),I=I1,I2)
C 4400          CONTINUE
4500          CONTINUE
C
C
C          WRITE P(Z) AND DP/DR (Z) ONTO FILES
          DO 4600 J=1,NR
          PZAPIN=P(1,J)
          PZAPOUT=P(NC,J)

```

```

C
      WRITE(7,*) ZC(J),PZAPIN,PZAPOUT
4600  CONTINUE
C
      CLOSE (2)
      CLOSE (3)
      CLOSE (6)
      CLOSE (7)
      STOP
10000 FORMAT(/,' ENTER INPUT FILE NAME: ',%)
10500 FORMAT(/,' NODAL MESH HAS ',I3,' COLUMNS (RADIAL COORDINATE)',/,
X      ' AND ',I3,' ROWS (DEPTH COORDINATE) ')
11000 FORMAT(/,' ENTER RADIAL AND VERTICAL NODE COORDINATES OF SENSOR: '
X      ',%)
11500 FORMAT(/,' SENSOR IS LOCATED AT:',/,
X      ' R = ',E12.4, ' m',/,
X      ' Z = ',E12.4, ' m',/)
12000 FORMAT(/,' READING FINITE DIFFERENCE MESH DATA FILE',/)
14000 FORMAT(/,' BEGIN SIMULATION',/,
X      ' ITERATED ALTERNATING DIRECTION IMPLICIT (IADI)',/,
X      ' FINITE DIFFERENCE METHOD',/)
16000 FORMAT(A)
18000 FORMAT(/,' ENTER OUTPUT FILE NAME: ',%)
20000 FORMAT(/,' ENTER NO. FREQUENCIES AND THE ',/,
X      ' NUMBER OF FREQUENCY INCREMENTS BETWEEN LISTINGS: ',%)
22000 FORMAT(/,' ENTER FMIN, FMAX, AND THE ',/,
X      ' MAXIMUM PRESSURE CHANGE PER NODE (Pa)',/,
X      ' TO CONVERGENCE: ',%)
26000 FORMAT(2E15.6,4I15)
28000 FORMAT(5E15.6)
30000 FORMAT(I15,2E15.6)
34000 FORMAT(/,' ENTER UPPER BOUNDARY PRESSURE AMPLITUDE (Pa): ',%)
36000 FORMAT('1',//,' PSEUDO 3D BAROMETRIC GAS FLOW MODEL',//,
X      ' THE INPUT PARAMETERS FOR THIS RUN ARE:',//,' FREQUENCY STEP:',
XT30,E15.4,' 1/Sec',/, ' ERROR LIMIT:', '30,E16.4, ' Pa',/,
X      ' VISCOSITY:',T30,E16.4, ' Pa-sec',/,
X      ' MEAN BAROMETRIC PRESSURE:',T30,E16.4, ' Pa')
38000 FORMAT(/,T5,' LAYER NO.',T20,' PERMEABILITY (sq.m.)',T45,
X      ' POROSITY',/)
40000 FORMAT(T5,IS,T20,E14.3,T45,E9.3)
42000 FORMAT(/, ' RADIAL COORDINATES',//,T5,' NODE NO.',
XT20,' DISTANCE (m)')
44000 FORMAT(T5,IS,T20,F10.2)
46000 FORMAT(/, ' VERTICAL COORDINATES',//,T5,' NODE NO.',
XT20,' LAYER NO.',T35,' DISTANCE (m)')
48000 FORMAT(T5,IS,T20,IS,T35,F10.2)
50000 FORMAT(/,' PRESSURE VS FREQUENCY OUTPUT FILE NAME? ',%)
55000 FORMAT(/,' PRESSURE VS DEPTH (OUTER BOUNDARY) OUTPUT FILENAME? ',
X      '%)
56000 FORMAT(2E15.4)
58000 FORMAT(' ISTEP=',I4,' ITER=',I4,' MAX DELTA P=',
XE12.4)
59000 FORMAT(5(E12.4,1X))
60000 FORMAT(/, ' FREQUENCY (1/hr) = ',E12.4,/,
X      ' [REAL,IMAGINARY] SENSOR PRESSURE (Pa) = ',2(E12.4,2X),/,

```

```

      X ' AMPLITUDE (Pa), PHASE (deg)J =          ',2(E12.4,2X),//)
62000 FORMAT('1 NODAL PRESSURES (Pa)',//,T5,'FREQUENCY= ',
      XF10.0,' 1/secs',/,T5,' PAVG= ',E15.4,' Pascals',/,T5,
      X'TOTAL VOLUME FLUX INTO WELL= ',E15.4,' cu.m.')
```

64000 FORMAT(' J=I= ',6(I2,10X))

66000 FORMAT(/,1X,I3,6E12.5)

END

FINITE DIFFERENCE CHIMNEY MODELS (FORWARD)

- (1) RCHAN: SETS UP REQUIRED DATA FILES FOR CHAN AND FCHAN
- (2) CHAN: TIME DOMAIN FORWARD CHIMNEY MODEL
- (3) FCHAN: FREQUENCY DOMAIN FORWARD CHIMNEY MODEL

FINITE DIFFERENCE CHIMNEY MODEL (FORWARD AND INVERSE)

(TIME DOMAIN)

```

C      ++++++
C      +////////////////////+
C      +//////////////////// TDCA - MODULE 1 //////////////////////+
C      +////////////////////+
C      ++++++
C
C      WRITTEN BY:
C      JONATHAN M. HANSON
C      HANSON & ASSOCIATES
C      1336 EMBASSY WAY
C      SALT LAKE CITY, UTAH 84108
C
C      APPLICATION:
C      TDCA (Time Domain Chimney Analysis) DOES BOTH FORWARD AND INVERSE
C      MODEL ANALYSIS FOR NUCLEAR CHIMNEYS.
C
C      FORWARD MODEL:
C      GIVEN A SURFACE BAROMETRIC PRESSURE RECORD IN TIME, AND THE
C      GEOMETRY AND FLOW PARAMETERS OF A CHIMNEY-FORMATION SYSTEM,
C      THE FORWARD MODEL COMPUTES THE PRESSURE RESPONSE AT ANY
C      PRESCRIBED LOCATION AT DEPTH, EITHER WITHIN THE CHIMNEY
C      OR WITHIN THE SURROUNDING FORMATION, OR AT THE BOUNDARY
C      SEPARATING THE TWO.
C
C      INVERSE MODEL:
C      GIVEN MEASURED SURFACE AND SUBSURFACE BAROMETRIC PRESSURE DATA IN
C      TIME, AND A GIVEN GEOMETRY (CHIMNEY RADIUS, FORMATION LAYERING,
C      ETC.), THE INVERSE MODEL WILL VARY THE CHIMNEY AND FORMATION FLOW
C      PARAMETERS (PERMEABILITY AND POROSITY) IN SUCH A MANNER AS TO
C      MINIMIZE THE RMS DIFFERENCE BETWEEN THE MEASURED AND PREDICTED
C      SUBSURFACE PRESSURE RECORD. A SET OF INITIAL, OR STARTING, VALUES
C      OF THE FLOW PARAMETERS IS REQUIRED. THE USER HAS A CHOICE OF
C      MONTE CARLO, GRID SEARCH, OR RIDGE REGRESSION NONLINEAR LEAST
C      SQUARES TECHNIQUES.
C      $DEBUG
C      $LARGE
C      $NOFLOATCALLS
C      PROGRAM TDCA
C
C      DIMENSION T(1000), PSURF(1000), PCAVR(1000), PCAVT(1000)
C      DIMENSION A(20), AEX(20), SIGMAA(20), DELTAA(20), JFR(20)
C      DIMENSION YFIT(500), SIGMAY(500), B(20), DB(20)
C      DIMENSION CHI(20,20), VAR(20,20), COR(20,20)
C      DIMENSION NV(10)
C
C      DIMENSION POR(10), POR2(10), PERM(10), PERM2(10), H(10)
C      DIMENSION RC(20), ZC(200)
C      CHARACTER*20 ITYPE, NTYPE, GTYPE, NSEA, TYPE(20)
C      CHARACTER*20 HNAME, RNAME, FNAME, COMP, PFLAG, QFLAG
C      CHARACTER*20 ZSENS
C
C      COMMON /ZAP/ JFR, NTERMS, NFREE, NPTS
C      COMMON /DAT/ PSURF, PCAVT, DT, ER, PAVG, PFLAG
C      COMMON /STUFF/ MSTART

```

```

COMMON/STUFF2/QFLAG
COMMON/GEOM/NLAYER, NV, AC, ZC, NR, NC, RMIN, IRAD, IDEP
COMMON/DER/LPTS

C
C
      PI=3.141592654
      TWOPI=2.*PI

C
C
      INITIALIZE PARAMETER INDICES
        DO 100 J=1,20
          JFR(J)=J
100      CONTINUE

C
      ID1=0
      ID2=0

C
      SET VALUES FOR GAS VISCOSITY (pa.sec) AND MEAN GAS PRESSURE (pa)
      VISC=2.0D-05
      PAVB=8.5D04

C
      USE DEFAULT INITIAL FORMATION PRESSURE (85 kPa) OR
      USE TIME-AVERAGED:
      (1) MEASURED SURFACE PRESSURE FOR FORWARD PROBLEM
      (2) MEASURED DOWNHOLE PRESSURE FOR INVERSE PROBLEM
      WRITE (ID2,20000)
      READ (ID1,70000) GTYPE

C
      ENTER CHIMNEY-FORMATION GEOMETRY, AND FORMATION FLOW PARAMETERS
C
300  WRITE (*,10000)
      READ (*,*,ERR=300) RMIN,RMAX
350  WRITE (*,11000)
      READ (*,*,ERR=350) NCHIM
400  WRITE (*,12000)
      READ (*,*,ERR=400) NLAYER
        DO 800 N=1,NLAYER

C
C      FORMATION PERMEABILITY, POROSITY, LAYER THICKNESS
500  WRITE (*,13000) N
      READ (*,*,ERR=500) PERM(N),POR(N),H(N)
      PERM(N)=9.86923E-13*PERM(N)

C
C      CHIMNEY PERMEABILITY, POROSITY
550  WRITE (*,14000)
      READ (*,*,ERR=550) PERM2(N),POR2(N)
      PERM2(N)=9.86923E-13*PERM2(N)

C
C      NUMBER OF VERTICAL NODES IN LAYER
600  WRITE (*,15000)
      READ (*,*,ERR=600) NV(N)
      IF (NV(N).LT.2) GO TO 600

C
      LOAD PERMEABILITIES AND POROSITIES INTO PARAMETER ARRAY
      A(4*N-3)=PERM(N)

```

```

      A(4*N-2)=PERM2(N)
      A(4*N-1)=POR(N)
      A(4*N)=POR2(N)
C
      800      CONTINUE
C
      COMPUTE NODAL COORDINATES
C
      DR=RMIN/(NCHIM-1)
C
      SET RADIAL COORDINATES FOR CHIMNEY
      DO 850 I=1,NCHIM
      RC(I)=FLOAT(I-1)*DR
      850 CONTINUE
      I=NCHIM
C
      SET RADIAL COORDINATES FOR FORMATION
      900 I=I+1
      RC(I)=DR*2.0**((I-1-NCHIM)+RMIN
      IF (RC(I)-RMAX) 900,1000,1000
      1000 RC(I)=RMAX
      NC=1
      D=0
      ZC(1)=0
      NR=1
      DO 1200 I=1,NLAYER
      DD=H(I)/NV(I)
      DO 1100 J=1,NV(I)
      D=D+DD
      NR=NR+1
      1100 ZC(NR)=D
      1200 NV(I)=NR
C
C
C
      PRINT OUT NODE LOCATIONS
      WRITE(*,13500)
      DO 1250 J=1,NC
      WRITE(*,13600) J,RC(J)
      1250 CONTINUE
      WRITE(*,13700)
      DO 1260 J=1,NR
      WRITE(*,13600) J,ZC(J)
      1260 CONTINUE
C
      READ NODE COORDINATES FOR LOCATION OF IN-CHIMNEY MEASUREMENT
      SENSOR (RADIAL, DEPTH)
      1210 WRITE(*,17000)
      READ(*,*) IRAD, IDEP
C
      WRITE LOCATION OF SENSOR
      WRITE(*,16000) RC(IRAD),ZC(IDEP)
C
      WRITE(*,16500)
      READ(*,70000) ZSENS

```

```

C      IF(ZSENS.EQ.'N') GOTO 1210
C
C      INPUT FINITE DIFFERENCE ITERATION CONVERGENCE CRITERION
C      WRITE (ID2,18000)
C      READ (ID1,*) ER
C
C      SPECIFY WHETHER OR NOT TO PRINT OUT COMPUTED PRESSURES
C      (EITHER IN FORWARD OR INVERSE CALCULATIONS) AT EACH
C      TIME STEP. NOTE: THIS INFO. WILL BE STORED ON A DISK FILE
C      ANYWAY...IF YOU DON'T WANT A LOT OF HARDCOPY, SPECIFY
C      NO!
C      WRITE(ID2,72000)
C      READ(ID1,70000) PFLAG
C
C      SPECIFY EITHER FORWARD OR INVERSE CALCULATION:
C      FORWARD: COMPUTE THEORETICAL PRESSURE RESPONSE IN THE TIME
C      DOMAIN GIVEN INPUT SYSTEM PARAMETERS.
C      INVERSE: COMPUTE SYSTEM PARAMETERS GIVEN THEORETICAL
C      PRESSURE RESPONSE IN THE TIME DOMAIN.
C
C      WRITE (ID2,32000)
C      READ (ID1,70000) NTYPE
C      IF (NTYPE.EQ.'I') GO TO 2100
C
C      ----- FORWARD SOLUTION -----
C
C      ENTER MEASURED SURFACE PRESSURE DATA FILENAME
C      WRITE (ID2,44000)
C      READ (ID1,70000) RNAME
C      OPEN (7, FILE=RNAME, STATUS='OLD')
C
C      ENTER PREDICTED DOWNHOLE PRESSURE DATA FILENAME
C      WRITE (ID2,44500)
C      READ (ID1,70000) FNAME
C      OPEN (8, FILE=FNAME, STATUS='NEW')
C
C      CHECK IF SURFACE DATA IS IN PSI OR PA
C      WRITE (ID2,19000)
C      READ (ID1,70000) ITYPE
C      IF (ITYPE.EQ.'PSI') CONV=6.8947E03
C      IF (ITYPE.EQ.'PA') CONV=1.0
C
C      ADD NOISE TO SYSTEM RESPONSE?
C      XNS=0.0
C      MODE=0
C      WRITE (ID2,53000)
C      READ (ID1,56000) NOIS
C      IF (NOIS.NE.'Y') GO TO 1400
C      MODE=1
C      WRITE (ID2,54000)
C      READ (ID1,*) XNS

```

```

C
1400 WRITE (ID2,21000)
      READ (ID1,*) NBUMP
C
C   READ DATA FROM INPUT DATA FILE
      MBUMP=0
      READ (7,*) NT
      NPTS=NT
      K=0
      SS=0.0
      DO 1500 J=1,NT
        READ (7,*) TT,PP
        MBUMP=MBUMP+1
        IF (MBUMP.NE,NBUMP) GO TO 1500
        K=K+1
        MBUMP=0
        T(K) =TT
        PSURF(K)=CONV*PP
        SS=SS+CONV*PP
1500   CONTINUE
C
      NPTS=K-1
      NT=NPTS
      PAVTOP=SS/FLOAT(NPTS)
      IF (GTYPE.EQ.'B') PAVG=PAVTOP
C
C
      NTERMS=4*NLAYER
      NVAR=NTERMS
      NFREE=NPTS-NTERMS
      NFR=NFREE
C
C   CONVERT DELTA TIME TO SECONDS
      DT=3600.*(T(2)-T(1))
C
C   COMPUTE THEORETICAL DOWNHOLE PRESSURE RESPONSE
      DO 1800 J=1,NT
        PCAVT(J)=FUNCTN(T,J,A)
1800   CONTINUE
C
C   STORE THEORETICAL PRESSURE RESPONSE ON FILE
      WRITE (8,*) NT
      DUMMY=.21289
      DO 2000 J=1,NT
        CALL RAN(DUMMY)
        ZIP=DUMMY
C   ADD NOISE (IF REQUESTED) AND CONVERT BACK TO ORIGINAL
C   PRESSURE UNITS
        PCAVT(J)=(PCAVT(J)+XNS*(ZIP-0.5))/CONV
        SIGMAY(J)=XNS
        WRITE (8,*) T(J),PCAVT(J)
2000   CONTINUE
C
      CLOSE (8,STATUS='KEEP')
C

```

```

      GO TO 5500
C
C      ----- END OF FORWARD SOLUTION -----
C
C      ----- INVERSE SOLUTION -----
C
C      OPEN MEASURED SURFACE PRESSURE DATA FILE
2100 WRITE (ID2,44000)
      READ (ID1,70000) RNAME
      OPEN (7, FILE=RNAME, STATUS='OLD')
C
C      OPEN MEASURED DOWNHOLE PRESSURE DATA FILE
      WRITE (ID2,45000)
      READ (ID1,70000) HNAME
      OPEN (8, FILE=HNAME, STATUS='OLD')
C
C      OPEN COMPUTED DOWNHOLE PRESSURE DATA FILE
      WRITE (ID2,44500)
      READ (ID1,70000) FNAME
      OPEN (9, FILE=FNAME, STATUS='NEW')
C
C      CHECK IF SURFACE DATA IS IN PSI OR PA
      WRITE (ID2,19000)
      READ (ID1,70000) GTYPE
      IF (GTYPE.EQ.'PSI') CONV=6.8947E03
      IF (GTYPE.EQ.'PA') CONV=1.0
C
C      SPECIFY MAXIMUM TIME
      WRITE (ID2,77000)
      READ (ID1,*) TMAX
C
C      READ TIME AND PRESSURE DATA
2150 WRITE (ID2,21000)
      READ (ID1,*) NBUMP
C
      READ (7,*) NT
      READ (8,*) NT
      NPTS=NT
      K=0
      MBUMP=0
      SS1=0.0
      SS2=0.0
C
      DO 2400 J=1,NT
      READ (7,*) TT1,PP1
      READ (8,*) TT2,PP2
      MBUMP=MBUMP+1
      IF (MBUMP.NE.NBUMP) GO TO 2400
      K=K+1
      MBUMP=0
      T(K)=TT2
      PSURF(K)=CONV*PP1
      PCAVR(K)=CONV*PP2
      SIGMAY(K)=XNS
      SS1=SS1+CONV*PP1

```



```

                SS2=SS2+CONV*FP2
                IF (T(K).GT.TMAX) GOTO 2450
2400      CONTINUE
C
2450      NPTS=K
          NT=NPTS
          WRITE(9,*) NPTS
          LPTS=NPTS
          DT=3600.*(T(2)-T(1))
          PAVTOP=SS1/FLOAT(K)
          PAVBOT=SS2/FLOAT(K)
          DELP=PAVBOT-PAVTOP
          IF (GTYPE.EQ.'B') PAVG=PAVBOT
C
C      REFERENCE PRESSURE MEASUREMENTS TO COMMON ELEVATION?
          WRITE(ID2,73000)
          READ(ID1,70000) ITYPE
          IF (ITYPE.NE.'Y') GOTO 2650
C
          WRITE(ID2,75000) PAVTOP,PAVBOT
C      ESTIMATE ELEVATION DIFFERENCE BETWEEN SURFACE SENSOR AND
C      IN-HOLE SENSOR
          DEPSENS=16000.*DELP/(PAVTOP+PAVBOT)
          WRITE(ID2,12500) DEPSENS
C
C      REFERENCE PRESSURE DATA (SURFACE AND DOWNHOLE) TO COMMON DEPTHS
          DO 2600 J=1,NPTS
            PSURF(J)=PSURF(J)+DELP
2600      CONTINUE
C
C      INPUT ESTIMATED UNCERTAINTY IN DATA
C      MODE=0...MEASURED DOWNHOLE DATA IS EXACT
C      MODE=1...MEASURED DOWNHOLE DATA HAS A "ONE-SIGMA" = UNCE
2650      WRITE (ID2,24000)
          READ (ID1,*) MODE
          IF (MODE.EQ.0) GO TO 2800
          WRITE (ID2,25000)
          READ (ID1,*) UNCE
          DO 2700 J=1,NPTS
            SIGMA(J)=UNCE
2700      CONTINUE
C
C      ENCODE PARAMETER SET
C      INPUT NO. FREE PARAMETERS IN MODEL
2800      WRITE (ID2,33000)
          READ (ID1,*) NFR
          NFREE=NPTS-NFR
          NFRP1=NFR+1
          NTERMS=4*NLAYER
C
C      SPECIFY WHICH PARAMETERS IN MODEL ARE FREE PARAMETERS...
C      IE. ALLOWED TO VARY TO FIT THE DATA
          DO 2900 J=1,NFR
            WRITE (ID2,34000) J
            READ (ID1,*) JFR(J)

```

```

                TYPE (J)='FREE'
2900    CONTINUE
C
C    ASSIGN REMAINDER OF ENCODED MODEL PARAMETERS
        DO 3000 J=NFRP1,NTERMS
            K=J-NFRP1+1
            WRITE (ID2,35000) K
            READ (ID1,*) JFR(J)
            TYPE (J)='FIXED'
3000    CONTINUE
C
C    SPECIFY VALUES OF FIXED MODEL PARAMETERS
        DO 3100 J=NFRP1,NTERMS
            A(J)=AEX(JFR(J))
3100    CONTINUE
C
C    SPECIFY STARTING VALUES OF FREE PARAMETERS
        DO 3200 J=1,NFR
            A(J)=AEX(JFR(J))
3200    CONTINUE
C
C    PRINT OUT MODEL PARAMETER SUMMARY
        WRITE (ID2,27000)
        DO 3300 J=1,NTERMS
            WRITE (ID2,28000) JFR(J),AEX(JFR(J)),TYPE(J)
C 3300    CONTINUE
C
C    ENTER BEGINNING TIME FOR WHICH DIFFERENCE BETWEEN MODEL AND
C    DATA IS TO BE MINIMIZED.
        WRITE (ID2,31000)
        READ (ID1,*) TST
C
C    DETERMINE STARTING INDEX FOR DATA-MODEL COMPARISON
        DO 3400 J=1,NPTS
            IF (T(J).GE.TST) GO TO 3500
3400    CONTINUE
3500    MSTART=J
        JPTS=NPTS-MSTART+1
C
C    DEFINE NUMBER OF DEGREES OF FREEDOM BASED ON NUMBER OF DATA
C    POINTS IN MODEL-DATA COMPARISON AND NUMBER OF FREE PARAMETERS
C    IN MODEL.
        NFREE=JPTS-NFR
C
        WRITE (ID2,50000)
        READ (ID1,70000) MC
C
        IF (MC.NE.'Y') GO TO 4100
C
C    ----- BEGIN MONTE CARLO SEARCH -----
C
        KOUNT=0
        TEMP=1.0E20
        NPRN=NTERMS/4
C    INPUT PARAMETER RANGE FOR MONTE CARLO SEARCH

```

```

        DO 3600 J=1,NFR
        WRITE (ID2,51000) JFR(J)
        READ (ID1,*) B1,B2
        B(J)=B1
        DB(J)=B2-B1
3600    CONTINUE
C
C    INPUT NO. TIMES DICE ARE TO BE THROWN
        WRITE (ID2,22000)
        READ (ID1,*) KMAX
        DUMMY=0.21289
C
C    THROW THE DICE
3700    DO 3800 J=1,NFR
        CALL RAN(DUMMY)
        A(J)=B(J)+DUMMY*DB(J)
3800    CONTINUE
C
        DO 3900 J=1,NPTS
        PCAVT(J)=FUNCTN(T,J,A)
3900    CONTINUE
C
        KOUNT=KOUNT+1
        IF (KOUNT.GT.KMAX) GO TO 5500
        CHISQR=FCHISQ(PCAVT, SIGMA, NPTS, NFREE, MODE, PCAVT)
        IF (CHISQR.GT.TEMP) GO TO 3700
        PROBAB=PCHISQ(CHISQR, NFREE)
C
        WRITE (ID2,63000) CHISQR
        WRITE (ID2,64000) PROBAB
        DO 4000 LL=1,NPRN
        KBOT=(LL-1)*4+1
        KTOP=LL*4
        IF (LL.EQ.NPRN) KTOP=NTERMS
        WRITE (ID2,62000)
        WRITE (ID2,58000) (JFR(K),K=KBOT,KTOP)
        WRITE (ID2,57000) (A(K),K=KBOT,KTOP)
4000    CONTINUE
C
        TEMP=CHISQR
        GO TO 3700
C
C ----- END OF MONTE CARLO SEARCH -----
C
C ----- BEGIN NON-LINEAR INVERSION -----
C
C    SET UP PARAMETERS FOR NON-LINEAR INVERSION
4100    NPTS=NT
        FLAMDA=0.001
C
C    SPECIFY FRACTION OF START VALUE TO BE INCREMENT
        WRITE (ID2,48000)
        READ (ID1,*) XFRAC
C
C    INITIALIZE PARAMETER INCREMENTS
        DO 4200 J=1,NFR

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                                DELTAA(J)=XFRAC*A(J)
4200      CONTINUE
C
C      SPECIFY PRECISION OF CHISQR MINIMUM
C      WRITE (ID2,69000)
C      READ (ID1,*) PRES
C
C      PRINT OUT A LIMITED HISTORY OF THE PARAMETER SEARCH.
C      THIS WILL ALLOW THE USER TO IDENTIFY AT ANY GIVEN TIME
C      DURING EXECUTION JUST EXACTLY WHERE THE INVERSION IS.
C      WRITE(ID2,76000)
C      READ(ID1,70000) QFLAG
C
C      SPECIFY EITHER MARQUARDT OR GRID SEARCH
C      WRITE (ID2,47000)
C      READ (ID1,70000) NSEA
C
C      WRITE HEADER
C      IF (NSEA.EQ.'M') WRITE (ID2,41000)
C      IF (NSEA.EQ.'G') WRITE (ID2,42000)
C
C      COMMENCE ITERATION SEQUENCE...STOP WHEN CHISQR IS MINIMUM
C      TEMP=1.0
C      DO 5200 J=1,200
C      WRITE (ID2,59000) J
C      IF (NSEA.EQ.'G') GO TO 4500
C      CALL CURFIT(T,PCAVR,SIGMAY,NPTS,NFR,MODE,A,DELTAA,VAR,FLAMDA,
X      PCAVT,CHISQR,NVAR)
C      DO 4400 K=1,NFR
C      SIGMAA(K)=SQRT(VAR(K,K))
C      DO 4300 L=1,K
C      COR(K,L)=SQRT(VAR(K,L)**2/(VAR(K,K)*VAR(L,L)))
4300      CONTINUE
4400      CONTINUE
C      GO TO 4600
4500      CALL GRIDLS(T,PCAVR,SIGMAY,NPTS,NFR,MODE,A,DELTAA,SIGMAA,
X      PCAVT,CHISQR)
C
C      PROBAB=PCHISQ(CHISQR,NFREE)
C      NPRN=NTERMS/4
C      IF (NTERMS.LT.4) NPRN=1
C
C      WRITE (ID2,63000) CHISQR
C      WRITE (ID2,64000) PROBAB
C      WRITE (ID2,62000)
C      DO 4700 LL=1,NPRN
C      KBOT=(LL-1)*4+1
C      KTOP=LL*4
C      IF (KTOP.GT.NTERMS) KTOP=NTERMS
C      MDIF=KTOP-KBOT+1
C      IF (MDIF.EQ.1) GOTO 4650
C      IF (MDIF.EQ.2) GOTO 4660
C      IF (MDIF.EQ.3) GOTO 4670
C      WRITE (ID2,58000) (JFR(K),K=KBOT,KTOP)
C      WRITE (ID2,57000) (A(K),K=KBOT,KTOP)

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        WRITE (ID2,61000) (SIGMAA(K),K=KBOT,KTOP)
        GOTO 4700
4650      WRITE (ID2,58003) (JFR(K),K=KBOT,KTOP)
        WRITE (ID2,57003) (A(K),K=KBOT,KTOP)
        WRITE (ID2,61003) (SIGMAA(K),K=KBOT,KTOP)
        GOTO 4700
4660      WRITE (ID2,58002) (JFR(K),K=KBOT,KTOP)
        WRITE (ID2,57002) (A(K),K=KBOT,KTOP)
        WRITE (ID2,61002) (SIGMAA(K),K=KBOT,KTOP)
        GOTO 4700
4670      WRITE (ID2,58001) (JFR(K),K=KBOT,KTOP)
        WRITE (ID2,57001) (A(K),K=KBOT,KTOP)
        WRITE (ID2,61001) (SIGMAA(K),K=KBOT,KTOP)
4700      CONTINUE
C
        WRITE (ID2,67000)
        IF (NSEA.EQ.'G') GO TO 5100
        WRITE (ID2,65000)
            DO 4800 K=1,NFR
            DO 4750 L=1,K
                WRITE (ID2,68000) K,L,COR(K,L)
4750          CONTINUE
4800          CONTINUE
        WRITE (ID2,67000)
            DO 5000 K=2,NFR
            DO 4900 L=1,K-1
                R=COR(K,L)
                CORREL=1.0-PCORRE(R,JPTS,NFR)
                WRITE (ID2,66000) JFR(K),JFR(L),CORREL
4900          CONTINUE
5000          CONTINUE
C
5100      WRITE (ID2,67000)
C
        RAT=ABS((TEMP-CHISQR)/TEMP)
        IF (RAT.LE.PRES) GO TO 5300
        TEMP=CHISQR
        WRITE (ID2,60000)
5200      CONTINUE
C
5300      DO 5400 J=1,NPTS
        WRITE (9,*) T(J),PCAVT(J)
5400      CONTINUE
5500      STOP
10000      FORMAT('      ENTER CHIMNEY RADIUS (m) AND OUTER RADIUS (m): ',/)
11000      FORMAT('      ENTER NO. RADIAL NODES IN CHIMNEY: ',/)
12500      FORMAT('      ELEVATION DIFFERENCE (m) BETWEEN SURFACE AND IN-HOLE',
X          ' SENSORS IS ',F5.2)
12000      FORMAT('      ENTER NO. LAYERS: ',/)
13000      FORMAT('      ENTER FORMATION K(d), PHI, AND THICKNESS FOR LAYER ',
X          ' I2, ',/,)
13500      FORMAT('      ---- RADIAL NODE SPACING ---- ',/,
X          '      RADIAL NODE INDEX      R(m) ',/,)
13600      FORMAT(8X,13,9X,F7.2)
13700      FORMAT('      ---- VERTICAL NODE SPACING ---- ',/,)

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X          'VERTICAL NODE INDEX      Z(m) ',//
14000 FORMAT(/, ' ENTER CHIMNEY K(d) AND PHI FOR THIS LAYER: ', $)
15000 FORMAT(/, ' ENTER NO. VERTICAL NODES IN LAYER: ', $)
16000 FORMAT(/, ' SENSOR LOCATED AT R= ', E12.4, /,
X          ' Z= ', E12.4, //)
16500 FORMAT(/, ' IS SENSOR LOCATION OK? (Y/N): ', $)
17000 FORMAT(/, ' ENTER NODE MESH COORDINATES (RADIAL, VERTICAL) FOR',
X          ' SENSOR LOCATION: ', $)
18000 FORMAT(/, ' ENTER FINITE DIFFERENCE CONVERGENCE CRITERIA (Pa): ', $)
19000 FORMAT(/, ' DATA IS PSI OR PA? (ENTER PSI OR PA): ', $)
20000 FORMAT(/, ' DEFAULT P0 (85kPa) = A, COMPUTED = B: ', $)
21000 FORMAT(/, ' READ EVERY Nth DATA POINT - ENTER N: ', $)
22000 FORMAT(/, ' NO. TIMES DICE ARE TO BE THROWN? (I4): ', $)
24000 FORMAT(/, ' DATA MEASUREMENT IS EXACT : 0, OTHERWISE : 1 : ', $)
25000 FORMAT(/, ' ENTER DATA UNCERTAINTY (Pa): ', $)
28000 FORMAT(/, I2, 5X, E12.4, 5X, A6)
31000 FORMAT(/, ' ENTER START TIME (Hrs.) FOR COMPARISON ',
X          ' BETWEEN MODEL AND DATA: ', $)
32000 FORMAT(/, ' FORWARD=F, INVERSE=I')
33000 FORMAT(/, ' ENTER NO. FREE PARAMETERS IN MODEL: ', $)
34000 FORMAT(/, ' ENTER MODEL PARAMETER CORRESPONDING TO FREE '
X' PARAMETER ', I2, ' : ', $)
35000 FORMAT(/, ' ENTER MODEL PARAMETER CORRESPONDING TO FIXED '
X' PARAMETER ', I2, ' : ', $)
41000 FORMAT(/, I1, ' RIDGE REGRESSION ITERATION SEQUENCE', //)
42000 FORMAT(/, I1, ' GRID SEARCH ITERATION SEQUENCE', //)
44000 FORMAT(/, ' ENTER MEASURED SURFACE PRESSURE DATA FILE NAME: ', $)
44500 FORMAT(/, ' ENTER PREDICTED DOWNHOLE PRESSURE DATA FILE NAME: ', $)
45000 FORMAT(/, ' ENTER MEASURED DOWNHOLE PRESSURE DATA FILE NAME: ', $)
47000 FORMAT(/, ' MARGUARDT=M, GRID=G : ', $)
48000 FORMAT(/, ' ENTER FRACTION OF INITIAL A TO BE DELTA-A: ', $)
50000 FORMAT(/, ' MONTE CARLO SEARCH? (Y/N): ', $)
51000 FORMAT(/, ' ENTER MIN, MAX VALUES FOR MODEL PARAMETER ', I2, ' : ', $)
53000 FORMAT(/, ' ADD NOISE TO COMPUTED SYSTEM RESPONSE? (Y/N): ', $)
54000 FORMAT(/, ' ENTER NOISE LEVEL (PRESSURE UNITS): ', $)
56000 FORMAT(A1)
57000 FORMAT(1H, 4(E11.4, 10X))
57001 FORMAT(1H, 3(E11.4, 10X))
57002 FORMAT(1H, 2(E11.4, 10X))
57003 FORMAT(1H, 1(E11.4, 10X))
58000 FORMAT(1H, 4(' MODEL PARAM.', I2, 5X), //)
58001 FORMAT(1H, 3(' MODEL PARAM.', I2, 5X), //)
58002 FORMAT(1H, 2(' MODEL PARAM.', I2, 5X), //)
58003 FORMAT(1H, 1(' MODEL PARAM.', I2, 5X), //)
59000 FORMAT(1X, ' ***** ITERATION ', I3, ' *****', //)
60000 FORMAT(1X, ' *****', //)
61000 FORMAT(1H, 4(' ', E11.4, ' '), 8X, //)
61001 FORMAT(1H, 3(' ', E11.4, ' '), 8X, //)
61002 FORMAT(1H, 2(' ', E11.4, ' '), 8X, //)
61003 FORMAT(1H, 1(' ', E11.4, ' '), 8X, //)
62000 FORMAT(1H, 15X, ' PARAMETERS AND UNCERTAINTIES', //)
63000 FORMAT(1H, /, ' REDUCED CHI-SQUARE = ', E12.4)
64000 FORMAT(1H, /, ' PROBABILITY OF CORRECT PARENT FUNCTION = ',
X E12.4, //)
65000 FORMAT(1H, 10X, ' FREE PARAMETER CORRELATION MATRIX', //)

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66000 FORMAT(1H, ' PROBABILITY THAT A(      ) IS CORRELATED WITH '
      X 'A(', I1, ') IS ', E12.4, /)
67000 FORMAT(1H )
68000 FORMAT(1H , 14X, I2, 2X, I2, 2X, F12.4)
69000 FORMAT(/, ' ENTER CONVERGENCE CRITERION')
70000 FORMAT(A)
72000 FORMAT(/, ' PRINT INFO. AT EACH TIME STEP? (Y/N)')
73000 FORMAT(/, ' REFERENCE SENSOR DATA TO COMMON ELEVATION? (Y/N)')
75000 FORMAT(/, ' AVERAGE MEASURED SURFACE PRESSURE IS ', E16.6, /,
      X      ' AVERAGE MEASURED DOWNHOLE PRESSURE IS ', E16.6)
76000 FORMAT(/, ' PRINT OUT LIMITED HISTORY OF INVERSION?(Y/N)')
77000 FORMAT(/, ' ENTER MAXIMUM TIME (hrs)')
      END
      FUNCTION FUNCTN(T, KK, AC)

C
C      DEFINITION OF VARIABLES
C
C      NSTEPS - NUMBER OF TIME STEPS
C      DELTA - SIZE OF TIME STEP (Secs)
C      ERROR - MAXIMUM ALLOWED CONVERGENCE ERROR (Pa)
C      NC - NUMBER OF NODAL COLUMNS
C      NR - NUMBER OF NODAL ROWS
C      P(I, J) - NODAL PRESSURE AT CURRENT TIME STEP (Pa)
C      PO(I, J) - NODAL PRESSURE AT PREVIOUS TIME STEP (Pa)
C      DL(I, J) - CHANGE IN PRESSURE FROM PREVIOUS TIME STEP (Pa)
C      SF(I, J) - STORAGE COEFFICIENT (POROSITY * NODAL AREA / MEAN
C      ABSOLUTE PRESSURE) (sq. m./Pa)
C      Q(I, J) - TRUE VOLUMETRIC FLUX per UNIT THICKNESS (cu. m./sec)
C      QT - TOTAL VOLUME INFUX INTO WELL (cu. m)
C      C(I, J, 1) - NODAL CONDUCTIVITY IN Y-DIRECTION (sq. meter/Pa-sec)
C      C(I, J, 2) - NODAL CONDUCTIVITY IN X-DIRECTION
C      PAVG - AVERAGE ATMOSPHERIC PRESSURE (Pa)
C      VIS - VISCOSITY OF FLUID (Pa-sec)
C      PERM(I) - PERMEABILITY OF LAYER I (sq. m.)
C      POR(I) - POROSITY OF LAYER I
C
      DIMENSION P(20, 200), PO(20, 200), SF(20, 200),
X C(20, 200, 2), DL(20, 200), RC(20), ZC(200), AD(20), AC(20)
      DIMENSION NV(10)
      DIMENSION B(200), G(200)
      DIMENSION PSURF(1000), PCAVT(1000), T(1000)
      CHARACTER*20 PFLAG

C
      COMMON /DAT/ PSURF, PCAVT, DT, ER, PAVG, PFLAG
      COMMON /GEOM/ NLayer, NV, RC, ZC, NR, NC, RMIN, IRAD, IDEP
      COMMON /ZAP/ JFR(20), NTERMS, NFREE, NPTS

C
      PI=3.14159265
      TWO=2.0
      TWOPI=TWO*PI
      VIS=2.0E-05
      DELTA=DT
      ERROR=ER

C
      IF(KK.GT.1) GOTO 4600

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```

C
C      DECODE PARAMETERS
DO 100 J=1, NTERMS
  AD(JFR(J))=AC(J)
100 CONTINUE
C
C      COMPUTE NODAL CONDUCTIVITIES AND STORAGE FACTORS
C
  L=1
  DO 300 J=1, NR
    IF (J.GT.NV(L)) L=L+1
    DZ=ZC(MIN0(J+1, NR))-ZC(MAX0(J-1, 1))
    DO 200 I=1, NC
      IF (I.GT.NCHIM) GOTO 1250
      CL=AD(4*L-2)/VIS
      SFL=AD(4*L)/PAVG
      GOTO 1260
1250    CL=AD(4*L-3)/VIS
      SFL=AD(4*L-1)/PAVG
1260    DR=RC(MIN0(I+1, NC))-RC(MAX0(I-1, 1))
      IF (I.NE.NC) C(I, J, 2)=CL*DZ/((RC(I+1)-RC(I))*2.0)
      IF (J.NE.NR) C(I, J, 1)=CL*DR/((ZC(J+1)-ZC(J))*2.0)
      SF(I, J)=SFL*DZ*DR/4.0
      PC(I, J)=PAVG
      P(I, J)=PAVG
200
C
C      SET BOUNDARY NODES
C
300    C(NC, J, 2)=0.0
C
C      SET NO-FLOW CONDITION AT BOTTOM BOUNDARY
DO 400 I=1, NC
400  C(I, NR, 1)=0.0
C
C      REFINED NODAL VALUES ON BOUNDARIES OF HORIZONTAL LAYERS
C
  IF (N_LAYER.EQ.1) GO TO 600
  DO 500 L=1, N_LAYER-1
    DO 500 I=1, NC
      C(I, NV(L), 1)=C(I, NV(L)+1, 1)
      C(I, NV(L), 2)=(C(I, NV(L)-1, 2)+C(I, NV(L)+1, 2))/2.0
500    SF(I, NV(L))=(SF(I, NV(L)-1)+SF(I, NV(L)+1))/2.0
C
C      CONVERT FOR RADIAL FLOW WIDTHS
C
600    DO 800 J=1, NR
      DO 700 I=2, NC-1
        C(I, J, 1)=C(I, J, 1)*(RC(I-1)+RC(I+1))*PI
        SF(I, J)=SF(I, J)*(RC(I-1)+RC(I+1))*PI
700    C(I, J, 2)=C(I, J, 2)*(RC(I)+RC(I+1))*PI
    C(NC, J, 1)=C(NC, J, 1)*(RC(NC-1)+0.75*(RC(NC)-RC(NC-1)))*TWOPI
    SF(NC, J)=SF(NC, J)*(RC(NC-1)+0.75*(RC(NC)-RC(NC-1)))*TWOPI
    SF(1, J)=SF(1, J)*RC(2)*PI/2.0
    C(1, J, 1)=C(1, J, 1)*0.25*RC(2)*PI
800    C(1, J, 2)=C(1, J, 2)*0.50*RC(2)*PI

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```

C      DO 1000 I=1,NC
1000  SF(I,1)=1.0E25
C
C      ZERO OUT B AND G ARRAYS
      DO 1100 J=1,MTOP
        B(J)=0.0
        G(J)=0.0
1100  CONTINUE
C
C      START OF SIMULATION
C
      TIME=0.0
      DO 4500 ISTEP=1,NPTS
        TIME=TIME+DELTA
        TLM=TIME/3600.
C
C      SET UPPER BOUNDARY PRESSURE EQUAL TO BAROMETRIC PRESSURE AT
C      CURRENT TIME
C
      DO 1300 I=1,NC
        PQ(I,1)=PSURF(ISTEP)
1300  P(I,1)=PSURF(ISTEP)
C
C      PREDICT PRESSURES FOR NEXT TIME INCREMENT
C
1500      DO 1700 I=1,NC
              DO 1700 J=1,NR
                IF (SF(I,J).GT.1.0E20) P(I,J)=PQ(I,J)
                D=P(I,J)-PQ(I,J)
                PQ(I,J)=P(I,J)
                F=1.0
1700          P(I,J)=P(I,J)+D*F
C
C      REFINE ESTIMATES OF PRESSURES BY IADI METHOD
C
      ITER=0
1800      E=0.0
          ITER=ITER+1
C
C      COLUMN CALCULATIONS
C
      DO 3000 II=1,NC
        I=II
        IF (MOD(ISTEP+ITER,2).EQ.1) I=NC-I+1
        DO 2000 J=1,NR
C
C      CALCULATE B AND G ARRAYS
C
          BB=SF(I,J)/DELTA
          DD=PQ(I,J)*SF(I,J)/DELTA
          IF (J-1) 1900,2000,1900
1900      AA=-C(I,J-1,1)
          BB=BB+C(I,J-1,1)

```

```

2000      IF (J-NR) 2100,2200,2100
2100      CC=-C(I,J,1)
          BB=BB+C(I,J,1)
2200      IF (I-1) 2300,2400,2300
2300      BB=BB+C(I-1,J,2)
          DD=DD+P(I-1,J)*C(I-1,J,2)
2400      IF (I-NC) 2500,2600,2500
2500      BB=BB+C(I,J,2)
          DD=DD+P(I+1,J)*C(I,J,2)
2600      W=BB
          IF (J-1) 2700,2700,2650
2650      W=BB-AA*B(J-1)
2700      B(J)=CC/W
          G(J)=DD/W
          IF (J-1) 2800,2800,2750
          G(J)=G(J)-AA*G(J-1)/W
2750
2800      CONTINUE
C
C      RE-ESTIMATE PRESSURES
C
          EN=ABS(P(I,NR)-G(NR))
          E=AMAX1(E,EN)
          P(I,NR)=G(NR)
          N=NR-1
2900      HA=G(N)-B(N)*P(I,N+1)
          EN=ABS(HA-P(I,N))
          E=AMAX1(E,EN)
          P(I,N)=HA
          N=N-1
          IF (N) 3000,3000,2900
3000      CONTINUE
C
C      ROW CALCULATIONS
C
      DO 4100 JJ=1,NR
      J=JJ
      IF (MOD(ISTEP+ITER,2).EQ.1) J=NR-J+1
          DO 3900 I=1,NC
          BB=SF(I,J)/DELTA
          DD=PD(I,J)*SF(I,J)/DELTA
          IF (J-1) 3100,3200,3100
3100      BB=BB+C(I,J-1,1)
          DD=DD+P(I,J-1)*C(I,J-1,1)
3200      IF (J-NR) 3300,3400,3300
3300      DD=DD+P(I,J+1)*C(I,J,1)
          BB=BB+C(I,J,1)
3400      IF (I-1) 3500,3600,3500
3500      BB=BB+C(I-1,J,2)
          AA=-C(I-1,J,2)
3600      IF (I-NC) 3700,3800,3700
3700      BB=BB+C(I,J,2)
          CC=-C(I,J,2)
3800      W=BB
          IF (I-1) 3850,3850,3840
3840      W=W-AA*B(I-1)

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```

3850      B(I)=CC/W
          G(I)=DD/W
          IF (I-1) 3900,3900,3860
3860      G(I)=G(I)-AA*G(I-1)/W
3900      CONTINUE
C
C      RE-ESTIMATE PRESSURES
C
          EN=ABS(P(NC,J)-G(NC))
          E=AMAX1(E,EN)
          P(NC,J)=G(NC)
          N=NC-1
4000      HA=G(N)-B(N)*P(N+1,J)
          EN=ABS(P(N,J)-HA)
          E=AMAX1(E,EN)
          P(N,J)=HA
          N=N-1
          IF (N) 4100,4100,4000
4100      CONTINUE
C
          IF (E.GT.ERROR) GO TO 1800
          IF(ITER.GT.100) WRITE(ID2,12000)
          IF(ITER.GT.100) STOP
          PCAVT(ISTEP)=P(IRAD,IDEF)
          IF(PFLAG.EQ.'N') GOTO 4500
          WRITE(ID2,10000) ISTEP,ITER,TLM,PSURF(ISTEP),PCAVT(ISTEP)
C
4500      CONTINUE
4600      FUNCTN=PCAVT(KK)
4700      RETURN
C
10000    FORMAT(1H,3X,2(I3,2X),F10.4,2X,2(F12.6,2X))
11000    FORMAT(///,3X,' ISTEP ITER TIME (hrs) PSURF (Pa) PCAVT (Pa)',/)
12000    FORMAT(1H,' MORE THAN 100 ITERATIONS IN FUNCTN...STOP',
X' EXECUTION')
C
C      END

```

```

C      ++++++
C      +//
C      +// TDCA (MODULE 2) //
C      +//
C      ++++++
C
C      UNLESS OTHERWISE STATED, ALL OF THE FOLLOWING SUBROUTINES
C      CAN BE FOUND IN:
C      "DATA REDUCTION AND ERROR ANALYSIS FOR THE PHYSICAL
C      SCIENCES", P.R. BEVINGTON, MCGRAW-HILL, 1969.
C
C      SUBROUTINE CURFIT(X,Y,SIGMAY,NPTS,NTERMS,MODE,A,DELTA,
C      X VAR,FLAMDA,YFIT,CHISQR,NVAR)
C      DOUBLE PRECISION ARRAY
C      DIMENSION X(1),Y(1),SIGMAY(1),A(1),DELTA(1),YFIT(1)
C      DIMENSION WEIGHT(1000),ALPHA(20,20),BETA(20),DERIV(20,1000),
C      X ARRAY(20,20),B(20),VAR(20,20)
C      CHARACTER*20 QFLAG
C
C      OPERATIONAL MODIFICATIONS TO BEVINGTON ARE INDICATED BY
C      ASTERISKS
C      *****
C      COMMON/STUFF/MSTART
C      COMMON/DER/LPTS
C      COMMON/STUFF2/QFLAG
C      *****
C      ID1=0
C      ID2=0
C
C      PURPOSE:
C      MAKE A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION
C
C      USAGE:
C      CALL CURFIT(X,Y,SIGMAY,NPTS,NTERMS,MODE,A,DELTA,
C      X SIGMA,FLAMDA,YFIT,CHISQR)
C
C      DESCRIPTION OF PARAMETERS
C      X      - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C      Y      - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE
C      SIGMAY  - ARRAY OF STANDARD DEVIATIONS FOR Y DATA POINTS
C      NPTS    - NUMBER OF PAIRS OF DATA POINTS
C      NTERMS  - NUMBER OF FREE PARAMETERS
C      MODE    - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
C      +1 (INSTRUMENTAL) WEIGHT(I)=1./SIGMAY(I)**2
C      0 (NO WEIGHTING) WEIGHT(I)=1.
C      -1 (STATISTICAL) WEIGHT(I)=1./Y(I)
C      A      - ARRAY OF PARAMETERS
C      DELTA  - ARRAY OF INCREMENTS FOR PARAMETERS A
C      VAR    - VARIANCE-COVARIANCE MATRIX FOR PARAMETERS A
C      FLAMDA  - PROPORTION OF GRADIENT SEARCH INCLUDED
C      YFIT   - ARRAY OF CALCULATED VALUES OF Y
C      CHISQR  - REDUCED CHI SQUARE FOR FIT
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C      FUNCTN(X,I,A)

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C      EVALUATES THE FITTING FUNCTION FOR THE ITH TERM
C      FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
C      EVALUATES REDUCED CHI SQUARE FOR FIT TO DATA
C      FDERIV(X,I,A,DELTAA,NTERMS,DERIV)
C      EVALUATES THE DERIVATIVES OF THE FITTING FUNCTION
C      FOR THE ITH TERM WITH RESPECT TO EACH PARAMETER
C      MATINV(AHRRAY,NTERMS,DET)
C      INVERTS A SYMMETRIC TWO-DIMENSIONAL MATRIX OF DEGREE NTERMS
C      AND CALCULATES ITS DETERMINANT
C
C      COMMENTS:
C      DIMENSION STATEMENT VALID FOR NTERMS UP TO 10
C      SET FLAMDA=0.001 AT BEGINNING OF SEARCH
C
C      NFREE= NPTS-NTERMS
C      IF (NFREE) 200,200,300
200 CHISQR=0.
C      GO TO 3300
C
C      EVALUATE WEIGHTS
C
C      300      DO 1000 I=1,NPTS
C              IF (MODE) 500,800,900
C              IF (Y(I)) 700,800,600
C              WEIGHT(I)=1./Y(I)
C              GO TO 1000
C              700      WEIGHT(I)=1./(-Y(I))
C              GO TO 1000
C              800      WEIGHT(I)=1.
C              GO TO 1000
C              900      WEIGHT(I)=1./SIGMAY(I)**2
1000      CONTINUE
C
C
C      EVALUATE ALPHA AND BETA MATRICES
C
C      *****
C      DO 1200 J=1,NTERMS
C          BETA(J)=0.
C          DO 1200 K=1,J
1200      ALPHA(J,K)=0.
C          IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTING INITIAL FORWARD ',
C      X 'MODEL'
C          DO 1300 K=1,NPTS
1300      YFIT(K)=FUNCTN(X,K,A)
C
C      EVALUATE CHISQUARE AT STARTING POINT
C
C      CHISQ1=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INITIAL REDUCED CHI-SQUARE IS ',
C      X CHISQ1
C
C
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' ENTERING FDERIV FROM CURFIT'

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      CALL FDERIV(X,1,A,DELTA,NTERMS,DERIV)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' CALCULATING ALPHA AND BETA ',
X ' ARRAYS'
      DO 1500 I=MSTART,NPTS
        DO 1500 J=1,NTERMS
          BETA(J)=BETA(J)+WEIGHT(I)*(Y(I)-YFIT(I))*DERIV(J,I)
          DO 1500 K=1,J
            ALPHA(J,K)=ALPHA(J,K)+WEIGHT(I)*DERIV(J,I)
            *DERIV(K,I)
1500      X
1600      CONTINUE
          DO 1800 J=1,NTERMS
            DO 1800 K=1,J
1800      ALPHA(K,J)=ALPHA(J,K)
C      *****
C
C      INVERT MODIFIED CURVATURE MATRIX TO FIND NEW PARAMETERS
C
2000      DO 2200 J=1,NTERMS
        DO 2100 K=1,NTERMS
          ARRAY(J,K)=ALPHA(J,K)/SQRT(ALPHA(J,J)*ALPHA(K,K))
2100      CONTINUE
2200      ARRAY(J,J)=1./FLAMDA
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INVERTING MATRIX "ARRAY"'
      CALL MATINV(ARRAY,NTERMS,DET)
      DO 2400 J=1,NVAR
        B(J)=A(J)
2400      CONTINUE
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' UPDATING FREE PARAMETERS'
      DO 2500 J=1,NTERMS
        DO 2500 K=1,NTERMS
          VAR(J,K)=ARRAY(J,K)/(SQRT(ALPHA(J,J)*ALPHA(K,K)))
          B(J)=B(J)+BETA(K)*VAR(J,K)
      IF(QFLAG.EQ.'Y') WRITE(ID2,5000) J,B(J)
2500      CONTINUE
C
C      IF CHI SQUARE INCREASED, INCREASE FLAMDA AND TRY AGAIN
C
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTE NEW FORWARD MODEL'
      DO 2700 I=1,NPTS
2700      YFIT(I)=FUNCTN(X,I,B)
      CHISQR=FCHISQ(Y,SIGMA,NPTS,NFREE,MODE,YFIT)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' REDUCED CHI-SQUARE IS ', CHISQR
      IF (CHISQ1-CHISQR) 2900,3000,3000
2900      FLAMDA=10.0*FLAMDA
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' CHI-SQUARE INCREASED...',
X ' INCREASE LAMBDA AND TRY AGAIN'
      GO TO 2000
C
C      EVALUATE PARAMETERS AND VARIANCE-COVARIANCE MATRIX
C
3000      DO 3200 J=1,NTERMS
        DO 3100 K=1,NTERMS
3100      VAR(J,K)=CHISQR*VAR(J,K)
3200      A(J)=B(J)

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      FLAMDA=FLAMDA/10.0
3300 RETURN
5000 FORMAT(1H,'NEW VALUE OF PARAMETER ',12,' IS ',E13.5)
      END

C
C   SUBROUTINE GRIDLS
C
C   PURPOSE
C       MAKE A GRID-SEARCH LEAST-SQUARES FIT TO DATA WITH A SPECIFIED
C       FUNCTION WHICH IS NOT LINEAR IN COEFFICIENTS
C
C   USAGE
C       CALL GRIDLS(X,Y,SIGMAY,NPTS,NTERMS,MODE,A,DELTA,A,SIGMAA,
C       YFIT,CHISQR)
C
C   DESCRIPTION OF PARAMETERS
C       X       - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C       Y       - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE
C       SIGMAY  - ARRAY OF STANDARD DEVIATIONS FOR Y DATA POINTS
C       NPTS    - NUMBER OF PAIRS OF DATA POINTS
C       NTERMS  - NUMBER OF PARAMETERS
C       MODE    - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
C                 +1 (INSTRUMENTAL) WEIGHT(I)=1.0/SIGMAY(I)**2
C                 0  (NO WEIGHTING) WEIGHT(I)=1.0
C                 -1 (STATISTICAL) WEIGHT(I)=1.0/Y(I)
C       A       - ARRAY OF PARAMETERS
C       DELTA,A - ARRAY OF INCREMENTS FOR PARAMETERS A
C       SIGMAA  - ARRAY OF STANDARD DEVIATIONS FOR PARAMETERS A
C       YFIT    - ARRAY OF CALCULATED VALUES OF Y
C       CHISQR  - REDUCED CHI SQUARE FOR FIT
C
C   SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C       FUNCTN(X,I,A)
C           EVALUATES THE FITTING FUNCTION FOR THE ITH TERM
C       FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
C           EVALUATES REDUCED CHI SQUARE FOR FIT TO DATA
C
C   COMMENTS
C       DELTA,A VALUES ARE MODIFIED BY THE PROGRAM
C
C   SUBROUTINE GRIDLS (X,Y,SIGMAY,NPTS,NTERMS,MODE,A,DELTA,A,
C   XSIGMAA,YFIT,CHISQR)
C
C       DIMENSION X(1),Y(1),SIGMAY(1),A(1),DELTA,A(1),SIGMAA(1),YFIT(1)
C       CHARACTER*20 QFLAG
C
C   OPERATIONAL MODIFICATIONS TO BEVINGTON ARE INDICATED BY
C   ASTERISKS
C   *****
C   COMMON/STUFF/MSTART
C   COMMON/STUFF2/QFLAG
C   *****
C   ID1=0
C   ID2=0
C

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```

NFREE=NPTS-NTERMS
FREE=NFREE
CHISQR=0.0
IF (NFREE) 2600,2600,200
200   DO 2100 J=1,NTERMS
      IF(QFLAG.EQ.'Y') WRITE(ID2,5000) J
C
C   EVALUATE CHI SQUARE AT FIRST TWO SEARCH POINTS
C
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTE INITIAL FORWARD MODEL'
      DO 400 I=1,NPTS
400   YFIT(I)=FUNCTN(X,I,A)
      CHISQ1=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INITIAL REDUCED CHI-SQUARE IS ',
X CHISQ1
      FN=0.0
      DELTA=DELTAA(J)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INCREMENT PARAMETER'
600   A(J)=A(J)+DELTA
      IF(QFLAG.EQ.'Y') WRITE(ID2,5010) J,A(J)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTING FORWARD MODEL'
      DO 700 I=1,NPTS
700   YFIT(I)=FUNCTN(X,I,A)
      CHISQ2=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' REDUCED CHI-SQUARE IS NOW ',CHISQ2
      IF (CHISQ1-CHISQ2) 1000,600,1300
C
C   REVERSE DIRECTION OF SEARCH IF CHI SQUARE IS INCREASING
C
C
1000  DELTA=-DELTA
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' CHI-SQUARE IS INCREASING...',
X ' REVERSE DIRECTION OF SEARCH'
      A(J)=A(J)+DELTA
      IF(QFLAG.EQ.'Y') WRITE(ID2,5010) J,A(J)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTING FORWARD MODEL'
      DO 1100 I=1,NPTS
1100  YFIT(I)=FUNCTN(X,I,A)
      SAVE=CHISQ1
      CHISQ1=CHISQ2
      CHISQ2=SAVE
C
C   INCREMENT A(J) UNTIL CHI SQUARE INCREASES
C
C
1300  FN=FN+1.0
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INCREMENT PARAMETER'
      A(J)=A(J)+DELTA
      IF(QFLAG.EQ.'Y') WRITE(ID2,5010) J,A(J)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTING FORWARD MODEL'
      DO 1400 I=1,NPTS
1400  YFIT(I)=FUNCTN(X,I,A)
      CHISQ3=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' REDUCED CHI-SQUARE IS NOW ',

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```

      X CHISQ3
      IF (CHISQ3-CHISQ2) 1600,1700,1700
1600    CHISQ1=CHISQ2
      CHISQ2=CHISQ3
      GO TO 1300

C
C    FIND MINIMUM OF PARABOLA DEFINED BY LAST THREE POINTS
C
C
1700    DELTA=DELTA*(1./(1.+(CHISQ1-CHISQ2)/(CHISQ3-CHISQ2))+0.5)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' UPDATE PARAMETER BASED ON LAST ',
X ' THREE POINTS'
      A(J)=A(J)-DELTA
      IF(QFLAG.EQ.'Y') WRITE(ID2,5010) J,A(J)
      SIGMAA(J)=DELTA*(J)*SQRT(2.0/(FREE*(CHISQ3-2.0*CHISQ2+CHISQ1)
X      ))
      DELTAA(J)=DELTA*(J)*FN/3.0
      IF(QFLAG.EQ.'Y') WRITE(ID2,5020) J
2100    CONTINUE

C
C    EVALUATE FIT AND CHI SQUARE FOR FINAL PARAMETERS
C
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' EVALUATE FINAL FORWARD PROBLEM'
      DO 2300 I=1,NPTS
2300    YFIT(I)=FUNCTN(X,I,A)
      CHISQR=FCHISQ(Y,SIGMAA,NPTS,NFREE,MODE,YFIT)
      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' FINAL REDUCED CHI-SQUARE IS ',
X CHISQR
      DO 2500 K=1,NTERMS
2500    SIGMAA(K)=SQRT(CHISQR)*SIGMAA(K)
2600    RETURN
5000    FORMAT(1H ,///,' BEGIN VARYING PARAMETER ',I2,' IN GRID SEARCH')
5010    FORMAT(1H , ' CURRENT VALUE OF PARAMETER ',I2,' IS ',E12.4)
5020    FORMAT(1H , ' END OF PARAMETER ',I2,' VARIATION')
      END
      SUBROUTINE FDERIV(X,I,A,DELTA,NTERMS,DERIV)
      DIMENSION X(1000),A(20),DELTA(20),DERIV(20,1000)
C      *****
      DIMENSION YFIT1(1000),YFIT2(1000)
      CHARACTER*20 QFLAG
C      *****
C
C    OPERATIONAL MODIFICATIONS TO BEVINGTON ARE INDICATED BY
C    ASTERISKS
C
C    *****
      COMMON/DER/LPTS
      COMMON/STUFF2/QFLAG
C    *****
C
C    PURPOSE:
C    EVALUATE DERIVATIVES OF FUNCTION FOR LEAST-SQUARES
C    SEARCH FOR ARBITRAY FUNCTION GIVEN BY FUNCTN
C
C    USAGE:
C    CALL FDERIV(X,I,A,DELTA,NTERMS,DERIV)

```

```

C
C      DESCRIPTION OF PARAMETERS
C      X          - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C      I          - INDEX OF DATA POINTS
C      A          - ARRAY OF PARAMETERS
C      DELTAA     - ARRAY OF PARAMETER INCREMENTS
C      NTERMS     - NUMBER OF PARAMETERS
C      DERIV      - DERIVATIVES OF FUNCTION
C
C      SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED
C      FUNCTN(X,I,A)
C          EVALUATES THE FITTING FUNCTION FOR THE ITH TERM
C      *****
C          DO 700 J=1,NTERMS
C
C      IF(QFLAG.EQ.'Y') WRITE(ID2,5000) J
C          DELTA=DELTAA(J)
C          AJ=A(J)
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' INCREMENT PARAMETER'
C          A(J)=AJ+DELTA
C
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTE FORWARD MODEL'
C          DO 200 K=1,LPTS
C              YFIT1(K)=FUNCTN(X,K,A)
200      CONTINUE
C
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' DECREMENT PARAMETER'
C          A(J)=AJ-DELTA
C
C      IF(QFLAG.EQ.'Y') WRITE(ID2,*) ' COMPUTE FORWARD MODEL'
C          DO 300 K=1,LPTS
C              YFIT2(K)=FUNCTN(X,K,A)
300      CONTINUE
C
C      400      A(J)=AJ
C
C      500      DO 600 K=1,LPTS
C          DERIV(J,K)=(YFIT1(K)-YFIT2(K))/(2.0*DELTAA(J))
C      600      CONTINUE
C      700      CONTINUE
5000  FORMAT(1H,' PARAMETER ',I2,' IN FDERIV')
C      *****
C      RETURN
C      END
C      FUNCTION FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
C      DOUBLE PRECISION CHISQ,WEIGHT
C
C      OPERATIONAL MODIFICATIONS TO BEVINGTION ARE INDICATED BY
C      ASTERISKS
C      *****
C      COMMON/STUFF/MSTART
C      *****
C      DIMENSION Y(1),SIGMAY(1),YFIT(1)
C
C      PURPOSE

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```

C      EVALUATE REDUCED CHI SQUARE FOR FIT TO DATA
C      FCHISQ=SUM((Y-YFIT)**2/SIGMA**2)/NFREE
C
C      USAGE
C      RESULT=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
C
C      DESCRIPTION OF PARAMETERS
C      Y          - ARRAY OF DATA POINTS
C      SIGMAY     - ARRAY OF STANDARD DEVIATIONS FOR DATA POINTS
C      NPTS       - NUMBER OF DATA POINTS
C      NFREE      - NUMBER OF DEGREES OF FREEDOM
C      MODE       - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
C                  - +1 (INSTRUMENTAL) WEIGHT(I)=1./SIGMAY(I)**2
C                  - 0 (NO WEIGHTING) WEIGHT(I)=1.
C                  - -1 (STATISTICAL) WEIGHT(I)=1./Y(I)
C
C      YFIT       - ARRAY OF CALCULATED VALUES OF Y
C
C
C      CHISQ=0.
C      IF (NFREE) 300,300,400
300  FCHISQ=0.
C      GO TO 1400
C
C      ACCUMULATE CHI SQUARE
C
C      *****
C      400      DO 1100 I=MSTART,NPTS
C      *****
C          IF (MODE) 600,900,1000
C      600      IF (Y(I)) 800,900,700
C      700      WEIGHT=1./Y(I)
C          GO TO 1100
C      800      WEIGHT=1./(-Y(I))
C          GO TO 1100
C      900      WEIGHT=1.
C          GO TO 1100
C      1000     WEIGHT=1./SIGMAY(I)**2
C      1100     CHISQ=CHISQ+WEIGHT*(Y(I)-YFIT(I))**2
C
C      DIVIDE BY NUMBER OF DEGREES OF FREEDOM
C
C      FREE=NFREE
C      FCHISQ=CHISQ/FREE
C      1400  RETURN
C      END
C      SUBROUTINE RAN(R)
C      FROM PEERLESS ENGINEERING SERVICE
C      PUBLISHED AND COPYRIGHTED BY JOHN WILEY AND SONS
C
C      THIS SUBROUTINE GENERATES A SEQUENCE OF NUMBERS WHICH ARE
C      RANDOMLY AND UNIFORMLY DISTRIBUTED OVER THE UNIT INTERVAL
C
C      BB=1

```

```

      P1=R*317.
      R=AMOD(P1,BB)
      RETURN
      END
      FUNCTION PCORRE(R,NPTS,NTERMS)
C
C      PURPOSE
C          EVALUATE PROBABILITY FOR NO CORRELATION BETWEEN TWO VARIABLES
C
C      DESCRIPTION OF PARAMETERS
C          R      - LINEAR CORRELATION COEFFICIENT
C          NPTS   - NUMBER OF DATA POINTS
C          NTERMS - NUMBER OF MODEL PARAMETERS
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C          GAMMA(X)
C              CALCULATES GAMMA FUNCTION FOR INTEGERS AND HALF-INTEGERS
C
C          DOUBLE PRECISION R2,TERM,SUM,FI,FNUM,DENOM
C
C          EVALUATE NUMBER OF DEGREES OF FREEDOM
      NFREE=NPTS-NTERMS
      IF (NFREE) 200,200,300
200  PCORRE=0.0
      GO TO 1800
300  R2=R**2
      IF (1.0-R2) 200,200,400
400  NEVEN=2*(NFREE/2)
      IF (NFREE-NEVEN) 500,500,1000
C
C      NUMBER OF DEGREES OF FREEDOM IS EVEN
500  IMAX=(NFREE-2)/2
      FREE=NFREE
      TERM=ABS(R)
      SUM=TERM
      IF (IMAX) 1800,700,800
700  PCORRE=1.0-TERM
      GO TO 1800
800      DO 900 I=1,IMAX
          FI=I
          FNUM=IMAX-I+1
          DENOM=2*I+1
          TERM=-TERM*R2*FNUM/FI
900      SUM=SUM+TERM/DENOM
      PCORRE=1.128379167*(GAMMA((FREE+1.0)/2.0)/GAMMA(FREE/2.0))
      PCORRE=1.0-PCORRE*SUM
      GO TO 1800
C
C      NUMBER OF DEGREES OF FREEDOM IS ODD
C
1000 IMAX=(NFREE-3)/2
      TERM=ABS(R)*DSQRT(1.0-R2)
      SUM=DATAN(R2/TERM)
      IF (IMAX) 1700,1300,1400
1300 SUM=SUM+TERM

```

```

      GO TO 1700
1400 SUM=SUM+TERM
      DO 1600 I=1,IMAX
      FNUM=2*I
      DENOM=2*I+1
      TERM=TERM*(1.0-R2)*FNUM/DENOM
1600 SUM=SUM+TERM
1700 PCORRE=1.0-0.6366197724*SUM
1800 RETURN
      END
      FUNCTION PCHISQ (CHISQR,NFREE)
C
C   PURPOSE
C       EVALUATE PROBABILITY FOR EXCEEDING CHI SQUARE
C
C   USAGE
C       RESULT = PCHISQ (CHISQ, NFREE)
C
C   DESCRIPTION OF PARAMETERS
C       CHISQR - COMPARISON VALUE OF REDUCED CHI SQUARE
C       NFREE - NUMBER OF DEGREES OF FREEDOM
C
C   SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C       GAMMA(X)
C       CALCULATES GAMMA FUNCTION FOR INTEGERS AND HALF-
C       INTEGERS
C
C   COMMENTS
C       CALCULATION IS APPROXIMATE FOR NFREE ODD AND CHI SQUARE
C       GREATER THAN 50
C
      DOUBLE PRECISION Z,TERM,SUM,FACT
      IF (NFREE) 200,200,300
200 PCHISQ=0.
      GO TO 1500
300 FREE=NFREE
      Z=CHISQR*FREE/2.
      NEVEN=2*(NFREE/2)
      IF (NFREE-NEVEN) 400,400,800
C
C       NUMBER OF DEGREES OF FREEDOM IS EVEN
C
400 IMAX=NFREE/2
      TERM=1.0D0
      SUM=0.0D0
      DO 600 I=1,IMAX
      FI=I
      SUM=SUM+TERM
      IF (ABS(TERM).GT.1.0E20) GOTO 650
600 TERM=TERM*Z/FI
650 FACT=0.0D0
      IF (DABS(Z).GT.70.0D0) GO TO 700
      FACT=DEXP(-Z)
700 PCHISQ=SUM*FACT
      GO TO 1500

```

```

C
C      NUMBER OF DEGREES OF FREEDOM IS ODD
C
  800 IF (Z-25) 1000,1000,900
  900 Z=CHISQR*(FREE-1.)/2.
      GO TO 400
1000 PWR=FREE/2.
      TERM=1.
      SUM=TERM/PWR
          DO 1300 I=1,1000
              FI=I
              TERM=-TERM*Z/FI
              SUM=SUM+TERM/(PWR+FI)
              IF (DABS(TERM/SUM)-0.00001) 1400,1400,1300
1300      CONTINUE
1400 PCHISQ=1.-(Z**PWR)*SUM/GAMMA(PWR)
1500 RETURN
      END
      FUNCTION GAMMA(X)

C
C      PURPOSE
C          CALCULATE THE GAMMA FUNCTION FOR INTEGERS AND HALF-
C          INTEGERS
C
C      USAGE
C          RESULT=GAMMA(X)
C
C      DESCRIPTION OF PARAMETERS
C          X - INTEGER OR HALF-INTEGER
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C          FACTOR(N)
C              CALCULATES N FACTORIAL FOR INTEGERS
C
C          DOUBLE PRECISION PROD,SUM,FI
C
C      INTEGERIZE ARGUMENT
C
C          N=X-0.25
C          XN=N
C          IF (X-XN-0.75) 400,400,300
C
C          ARGUMENT IS INTEGER
C
  300 GAMMA=FACTOR(N)
      GO TO 1200
C
C          ARGUMENT IS HALF-INTEGER
C
  400 PROD=1.77245385
      IF (N) 800,800,500
  500 IF (N-10) 500,600,900
  600      DO 700 I=1,N
          FI=I
  700      PROD=PROD*(FI-0.5)

```

```

800 GAMMA=PROD
   GO TO 1200
900 SUM=0.0
      DO 1000 I=11,N
        FI=I
1000   SUM=SUM+DLOG(FI-0.5)
      IF (SUM.GE.71.78) SUM=71.78
      GAMMA=PROD*639383.8623*DEXP(SUM)
1200 RETURN
      END
      FUNCTION FACTOR(N)

C
C   PURPOSE
C       CALCULATES FACTORIAL FUNCTION FOR INTEGERS
C
C   DESCRIPTION OF PARAMETERS
C       N - INTEGER ARGUMENT
C
C       DOUBLE PRECISION FI,SUM
C       FACTOR=1.
C       IF (N-1) 800,800,200
200 IF (N-10) 300,300,500
C
C       N LESS THAN 11
C
C       DO 400 I=2,N
        FI=I
400   FACTOR=FACTOR*FI
      GO TO 800
C
C       N GREATER THAN 10
C
500 SUM=0.0
      DO 600 I=11,N
        FI=I
600   SUM=SUM+DLOG(FI)
      FACTOR=3628800.*DEXP(SUM)
800 RETURN
      END
      SUBROUTINE MATINV(ARRAY,NORDER,DET)

C
C   PURPOSE
C       INVERT A SYMMETRIC MATRIX AND CALCULATE ITS DETERMINANT
C
C   DESCRIPTION OF PARAMETERS
C       ARRAY - INPUT MATRIX WHICH IS REPLACED BY ITS INVERSE
C       NORDER - DEGREE OF MATRIX (ORDER OF DETERMINANT)
C       DET - DETERMINANT OF INPUT MATRIX
C
C   COMMENTS
C       DIMENSION STATEMENT VALID FOR NORDER UP TO 10
C
      DOUBLE PRECISION ARRAY,AMAX,SAVE
      DIMENSION ARRAY(20,20),IK(20),JK(20)
      DET=1.

```

```

      DO 2500 K=1,NORDER
C
C      FIND LARGEST ELEMENT ARRAY(I,J) IN REST OF MATRIX
C
      AMAX=0.
      300      DO 600 I=K,NORDER
                DO 600 J=K,NORDER
                  IF (DABS(AMAX)-DABS(ARRAY(I,J))) 500,500,600
      500      AMAX=ARRAY(I,J)
                IK(K)=I
                JK(K)=J
      600      CONTINUE
C
C      INTERCHANGE ROWS AND COLUMNS TO PUT AMAX IN ARRAY(K,K)
C
      IF (AMAX) 900,800,900
      800      DET=0.
      GO TO 3300
      900      I=IK(K)
      IF (I-K) 300,1200,1000
      1000     DO 1100 J=1,NORDER
                SAVE=ARRAY(K,J)
                ARRAY(K,J)=ARRAY(I,J)
      1100     ARRAY(I,J)=SAVE
      1200     J=JK(K)
      IF (J-K) 300,1500,1300
      1300     DO 1400 I=1,NORDER
                SAVE=ARRAY(I,K)
                ARRAY(I,K)=ARRAY(I,J)
      1400     ARRAY(I,J)=SAVE
C
C      ACCUMULATE ELEMENTS OF INVERSE MATRIX
C
      1500     DO 1700 I=1,NORDER
                IF (I-K) 1600,1700,1600
      1600     ARRAY(I,K)=-ARRAY(I,K)/AMAX
      1700     CONTINUE
      DO 2100 I=1,NORDER
                DO 2100 J=1,NORDER
                  IF (I-K) 1900,2100,1900
      1900     IF (J-K) 2000,2100,2000
      2000     ARRAY(I,J)=ARRAY(I,J)+ARRAY(I,K)*ARRAY(K,J)
      2100     CONTINUE
      DO 2400 J=1,NORDER
                IF (J-K) 2300,2400,2300
      2300     ARRAY(K,J)=ARRAY(K,J)/AMAX
      2400     CONTINUE
      ARRAY(K,K)=1./AMAX
      2500     DET=DET*AMAX
C
C      RESTORE ORDERING OF MATRIX
C
      DO 3200 L=1,NORDER
        K=NORDER-L+1
        J=IK(K)

```



```

                IF (J-K) 2900,2900,2700
2700            DO 2800 I=1,NORDER
                SAVE=ARRAY(I,K)
                ARRAY(I,K)=-ARRAY(I,J)
2800            ARRAY(I,J)=SAVE
2900            I=JK(K)
                IF (I-K) 3200,3200,3000
3000            DO 3100 J=1,NORDER
                SAVE=ARRAY(K,J)
                ARRAY(K,J)=-ARRAY(I,J)
3100            ARRAY(I,J)=SAVE
3200            CONTINUE
3300 RETURN
            END

```

CODE MODULE DRIVERS:

(1) DRIVER1: LINK WITH TIME-DOMAIN MODULES

(2) DRIVER2: LINK WITH FREQUENCY-DOMAIN MODULES

***** LISTINGS NOT GIVEN DUE TO EXCESSIVE LENGTH *****

(CODES WILL BE SUPPLIED TO LLNL ON FLOPPY DISKETTE)

APPENDIX II

Exerpt from:

Selected Digital Computer Techniques
for Groundwater Resource Evaluation

By:

T.A. Prickett and C.G. Lonnquist

Illinois State Water Survey
Urbana, Bull. 55, 1971

Selected Digital Computer Techniques for Groundwater Resource Evaluation

by T. A. PRICKETT and C. G. LONNGQUIST

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Title: Selected Digital Computer Techniques for Groundwater Resource Evaluation.

Abstract: Generalized digital computer program listings are given that can simulate one-, two-, or three-dimensional nonsteady flow of groundwater in heterogeneous aquifers under water table, nonleaky, and leaky artesian conditions. Included are listings for time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, and the mechanism of converting from artesian to water table conditions. Discussion includes necessary mathematical background, documented program listings, sample input data, job setup procedures, theoretical versus computer comparisons, and field examples. A finite difference approach is used to formulate the equations of groundwater flow; a modified alternating direction implicit method solves the set of resulting finite difference equations. Programs are written in FORTRAN IV and will operate with any consistent set of units. The digital computers can deal with much more complex problems than is practical with electric analog or analytical methods.

Reference: Prickett, T. A., and C. G. Lonngquist. Selected Digital Computer Techniques for Groundwater Resource Evaluation. Illinois State Water Survey, Urbana, Bulletin 55, 1971.

Indexing Terms: Case histories, digital computers, finite difference theory, groundwater, groundwater evapotranspiration, induced infiltration, leakage, models, numerical analysis, program listings, recharge, three-dimensional flow, variable pumpage.

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Selected Digital Computer Techniques for Groundwater Resource Evaluation

by T. A. Prickett and C. G. Lonquist

ABSTRACT

Generalized digital computer program listings are given that can simulate one-, two-, and three-dimensional nonsteady flow of groundwater in heterogeneous aquifers under water table, nonleaky, and leaky artesian conditions. Programming techniques involving time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, and the mechanism of converting from artesian to water table conditions are also included.

The discussion of the digital techniques includes the necessary mathematical background, documented program listings, theoretical versus computer comparisons, and field examples. Also presented are sample computer input data and explanations of job setup procedures.

A finite difference approach is used to formulate the equations of groundwater flow. A modified alternating direction implicit method is used to solve the set of resulting finite difference equations.

The programs included are written in FORTRAN IV and will operate with any consistent set of units.

INTRODUCTION

The use of digital computers in groundwater resource evaluation has grown rapidly within the past few years. Computers are now widely available that allow solution of large sets of simultaneous equations that are involved in studying cause and effect relationships in heterogeneous aquifer systems with a wide variety of boundary conditions. The digital computer can deal with problems of much greater complexity than is practical with electric analog or analytical methods. However, digital computers will not cause analytical methods or electric analog simulators to become obsolete; used in conjunction with these other tools available to the hydrologist, digital computers can greatly improve the analysis of groundwater problems.

This report, which describes the digital computer techniques used at this time by the Illinois State Water Survey, is aimed primarily to the engineer and geologist involved in evaluating groundwater resources. The discussion of the digital techniques includes the necessary mathematical background, documented program listings, theoretical examples, and field applications.

The main object of this report is to present generalized computer programs that will simulate one-, two-, or three-dimensional nonsteady-state flow problems in heterogeneous aquifers under water table, nonleaky, and leaky artesian conditions. These programs cover time varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapo-

transpiration, the mechanism of possible conversion of storage coefficients from artesian to water table conditions, and the three-dimensional problem.

A finite difference approach that is identical to that taken in designing electric analog simulators has been adopted in formulating the equations of groundwater flow. Thus investigators whose experience is solely with designing electric analogs will find many similarities in the digital model designing procedures.

Part 1 of this report provides a description of the mathematical derivation of the finite difference equations governing the flow of groundwater in a form amenable to digital computer solution. Also described is a modified alternating direction implicit procedure by which the computer programs solve the set of finite difference equations.

Part 2 presents a 'basic aquifer simulation program' and describes its use in detail. The basic aquifer simulation program is intended for studying cause and effect relationships in heterogeneous aquifer systems with constant pumpage taking place from wells simulated at any node point of the digital model.

The basic aquifer simulation program forms the nucleus of all remaining programs of the report. Part 3 includes the various modifications made to the basic program that allow incorporating additional features such as specialized types of printout and the differing boundary conditions mentioned above. The program modifications are added and discussed one at a time. The modified program listings

are given, sample data sets are included along with job setup instructions, and comparisons are made between theoretical and field examples where possible.

It is intended that simulation of various conditions, applicable for particular aquifer situations, can be accomplished by combining separate features of several computer programs. Given as an example is a combined aquifer simulation program that can simultaneously handle all of the conditions mentioned earlier.

Also included are a specialized computer model for a field example, an analog-digital computer comparison of solutions of a hypothetical model problem, and an analysis of heads or drawdowns at pumped well nodes of the digital model.

The computer programs included in this report were written in FORTRAN IV for use on an IBM 360 system model 75 with a G level compiler. However, the programs will operate, with modifications, on other computers. Also, these computer programs are written so that they will operate with any consistent set of units.

The reader should be cautioned that the program listings of this report are not intended to be 'canned programs' but are meant to present the basic concepts of individual boundary condition modeling which, in combination with one

another, will serve as a basis for designing digital models for particular aquifer situations.

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Part 1. Mathematical Background

Mathematical Derivation of Finite Difference Equations

The partial differential equation (Bittenger et al., 1967) governing the nonsteady-state, two-dimensional flow of groundwater in an artesian, nonhomogeneous, and isotropic aquifer is

$$\partial/\partial x (T \partial h/\partial x) + \partial/\partial y (T \partial h/\partial y) = S \partial h/\partial t + Q \quad (1)$$

where

T = aquifer transmissivity

h = head

t = time

S = aquifer storage coefficient

Q = net groundwater withdrawal rate per unit area

x, y = rectangular coordinates

There is no general solution to equation 1; however, a numerical solution of that equation can be obtained through a finite difference approach. The finite difference approach first involves replacing the continuous aquifer system parameters by an equivalent set of discrete elements. In working with digital computers both the space and time variables are treated as discrete parameters. Secondly, the equations governing the flow of groundwater in the discretized model are written in finite difference form. Finally, the resulting set of finite difference equations is solved numerically with the aid of a digital computer.

The finite difference equations can be derived in two ways; i.e., from the physical standpoint involving Darcy's law and the principle of conservation of mass, or by a conventional mathematical treatment, substituting finite difference approximations for the derivatives of equation 1. Both derivational routes lead to the same result. The finite difference equations of this report are derived from the physical standpoint as follows.

A finite difference grid is superposed over a map of an aquifer as illustrated in figure 1. The aquifer is thus subdivided into volumes having dimensions $m\Delta x\Delta y$ where m is the thickness of the aquifer. The differentials ∂x and ∂y are approximated by the finite lengths Δx and Δy , respectively. The area $\Delta x\Delta y$ should be small compared with the total area of the aquifer to the extent that the discrete model is a reasonable representation of the continuous system. The intersections of grid lines are called nodes and are referenced with a column (i) and row (j) coordinate system colinear with the x and y directions, respectively.

Flow rate terms ($Q_1, 2, 3, \dots, 6$) are arbitrarily assigned flow directions as illustrated in figure 1. Flow rate terms Q_1, Q_2, Q_3 , and Q_4 represent node-to-node water transfer rates. Q_5 is the flow rate associated with the amount of water taken into or released from storage per unit time increment Δt . Water is being taken into storage since the assigned direction of the flow rate term Q_5 is out of the node i,j as il-

Figure 1. Finite difference grid

lustrated in figure 1. Q_5 is defined as a net constant withdrawal rate. A seventh generalized flow rate term Q_7 is included to account for other special conditions such as leakage, induced infiltration, and effects of evapotranspiration which will be added later in this report.

The continuity condition relating the flow rates entering and leaving the node i,j of figure 1 requires that the rates be equal as follows

$$Q_5 + Q_1 + Q_2 = Q_3 + Q_4 + Q_6 \quad (2)$$

Determining the values of the flow rate terms of equation 2 involves three considerations. First, it is necessary to define what portion of the aquifer is represented by each individual term. Secondly, it must be kept in mind that, although the flow rates may take place in any direction in the aquifer system, they are restricted to the x and y directions in the finite difference approach. The portions of the aquifer included in the flow rate terms then may be referred to as 'vector volumes' to emphasize that not only a volume but also the direction of flow is being considered (Karpf, 1958). Finally, since time is discretized, equation 2 represents an instantaneous balance at the end of a time increment.

Horizontal projections of the vector volumes of the node-to-node flow rate terms Q_1, Q_2, Q_3 , and Q_4 are defined as illustrated in figure 2. All vector volumes of figure 2 have a vertical dimension extending the full depth of the aquifer, m . Furthermore, the portion of aquifer involved with each of these flow rate terms extends in width one half of the grid interval on either side of the line between node points.

Figure 2. Vector volumes for node-to-node flow rate terms

and is equal in length to the grid interval. Darcy's law is then applied to the flow rate terms Q_1 through Q_4 to give

$$Q_1 = T_{i-1,j} (h_{i-1,j} - h_{i,j}) \Delta y / \Delta x \quad (3a)$$

$$Q_2 = T_{i,j} (h_{i,j} - h_{i+1,j}) \Delta y / \Delta x \quad (3b)$$

$$Q_3 = T_{i,j+1} (h_{i,j+1} - h_{i,j}) \Delta x / \Delta y \quad (3c)$$

$$Q_4 = T_{i,j-1} (h_{i,j} - h_{i,j-1}) \Delta x / \Delta y \quad (3d)$$

where

$T_{i-1,j}$ = aquifer transmissivity within the vector volume between nodes i,j and $i,j+1$ (see figures 2c and d)

$T_{i,j}$ = aquifer transmissivity within the vector volume between nodes i,j and $i,j+1$ (see figures 2e and b)

$h_{i,j}$ = calculated heads at the end of a time increment measured from an arbitrary reference level at node i,j

Horizontal projections of the vector volumes of the flow terms Q_3 , Q_4 , and Q_5 are identical (figure 3). These vector volumes, except that related to Q_5 , extend the full depth of the aquifer and have horizontal dimensions of $\Delta x \Delta y$, the volumes being centered around the node point i,j .

The flow rate term Q_5 , representing the rate at which water is taken into storage, is given by

$$Q_5 = S \Delta x \Delta y (h_{i,j} - h\phi_{i,j}) / \Delta t \quad (4)$$

where

$h\phi_{i,j}$ = calculated head at node i,j at the end of the previous time increment Δt

Δt = time increment elapsed since last calculation of heads

Figure 3. Vector volumes for flow rate terms Q_1 , Q_2 , and Q_5

The flow rate term Q_5 is made equal to a constant net withdrawal rate from the vector volume of node i,j of figure 3 as follows

$$Q_5 = Q_{5,i} \quad (5)$$

Since no special source or sink functions are included at this time, the flow rate term Q_5 is set equal to zero. However, the term Q_5 will be carried along in the derivations that follow so that when special functions are included their relationships may be substituted without re-derivation. Therefore

$$Q_5 = Q_{5,i} \quad (6)$$

Substitution of equations 3, 4, 5, and 6 into equation 2 results in

$$Q_5 + T_{i-1,j} (h_{i-1,j} - h_{i,j}) \Delta y / \Delta x + T_{i,j+1} (h_{i,j+1} - h_{i,j}) \Delta x / \Delta y \\ = T_{i,j} (h_{i,j} - h_{i+1,j}) \Delta y / \Delta x + T_{i,j-1} (h_{i,j} - h_{i,j-1}) \Delta x / \Delta y \\ + S \Delta x \Delta y (h_{i,j} - h\phi_{i,j}) / \Delta t + Q_{5,i} \quad (7)$$

Dividing both sides of equation 7 by the product of $\Delta x \Delta y$ and rearranging terms yields

$$T_{i-1,j} (h_{i-1,j} - h_{i,j}) / \Delta x^2 + T_{i,j+1} (h_{i,j+1} - h_{i,j}) / \Delta y^2 \\ + T_{i,j} (h_{i,j} - h_{i+1,j}) / \Delta y^2 + T_{i,j-1} (h_{i,j} - h_{i,j-1}) / \Delta x^2 \\ = S (h_{i,j} - h\phi_{i,j}) / \Delta t + Q_{5,i} / \Delta x \Delta y - Q_{5,i} / \Delta x \Delta y \quad (8)$$

With $Q_{5,i}$ equal to zero, equation 8 is the finite difference form of the partial differential equation (see equation 1) governing the nonsteady-state, two-dimensional flow of groundwater in an artesian, nonhomogeneous aquifer. A similar equation was derived in a more formal manner by Pinder and Bredehoeft (1968, equation 20).

Since there is an equation of the same form as equation 8 for every node of the digital model, a large set of simultaneous equations must be solved for the principal unknowns $h_{i,j}$. A modified form of the alternating direction implicit

method of Peaceman and Rachford (1955), as described below, is used to solve the set of simultaneous equations.

Iterative Alternating Direction Implicit Method

Briefly, the iterative alternating direction implicit method involves first, for a given time increment, reducing a large set of simultaneous equations down to a number of small sets. This is done by solving the node equations by Gauss elimination of an individual column of the model while all terms related to the nodes in adjacent columns are held constant. According to Peaceman and Rachford (1955), the set of column equations is then implicit in the direction along the column and explicit in the direction orthogonal to the column alignment. The solution of the set of column equations is then a straightforward process which will be explained in the next section.

After all column equations have been processed column by column, attention is focused on solving the node equations again by Gauss elimination of an individual row while all terms related to adjacent rows are held constant. Finally, after all equations have been solved row by row, an 'iteration' has been completed. The above process is repeated a sufficient number of times to achieve convergence, and this completes the calculations for the given time increment. The calculated heads are then used as initial conditions for the next time increment. This total process is repeated for successive time increments. Peaceman and Rachford (1955) point out that this technique is unconditionally stable regardless of the size of the time increment.

Equation 8 is modified and rearranged to facilitate node equation solving by columns and rows. First it is assumed that the finite difference grid is made up of squares such that $\Delta y = \Delta x$. (The case where Δy does not equal Δx will be treated later in this report.) Equation 8 can then be rewritten by multiplying both sides by Δx^2 as follows:

$$\begin{aligned} T_{i-1,j} (h_{i-1,j} - h_{i,j}) + T_{i,j} (h_{i,j} - h_{i+1,j}) \\ + T_{i,j+1} (h_{i,j+1} - h_{i,j}) + T_{i,j-1} (h_{i,j-1} - h_{i,j}) \\ = (S\Delta x^2/\Delta t) (h_{i,j} - h\phi_{i,j}) + Q_{i,j} - Q_a \end{aligned} \quad (9)$$

Equation 9 is expanded, the signs are reversed, and terms of $h_{i,j}$ are grouped together to yield

$$\begin{aligned} h_{i,j} (T_{i-1,j} + T_{i,j} + T_{i,j+1} + T_{i,j-1} + S\Delta x^2/\Delta t) \\ - T_{i-1,j} h_{i-1,j} - T_{i,j} h_{i+1,j} - T_{i,j+1} h_{i,j+1} \\ - T_{i,j-1} h_{i,j-1} = (S\Delta x^2/\Delta t) h\phi_{i,j} - Q_{i,j} + Q_a \end{aligned} \quad (10)$$

Equation 10 is then written in two forms, one for solving the node equations by columns and the other for solving the node equations by rows.

For calculations by *columns*, equation 10 is rearranged as follows

$$\begin{aligned} -T_{i-1,j} h_{i-1,j} + h_{i,j} (T_{i-1,j} + T_{i,j} + T_{i,j+1} + T_{i,j-1} \\ + S\Delta x^2/\Delta t) - T_{i,j} h_{i+1,j} = (S\Delta x^2/\Delta t) h\phi_{i,j} - Q_{i,j} \\ + T_{i,j+1} h_{i,j+1} + T_{i,j-1} h_{i,j-1} + Q_a \end{aligned} \quad (11)$$

Equation 11 is of the form

$$AA_i h_{i-1,j} + BB_i h_{i,j} + CC_i h_{i+1,j} = DD_i \quad (11')$$

where the constant terms are

$$AA_i = -T_{i-1,j} \quad (11a)$$

$$BB_i = T_{i-1,j} + T_{i,j} + T_{i,j+1} + T_{i,j-1} + S\Delta x^2/\Delta t \quad (11b)$$

$$CC_i = -T_{i,j} \quad (11c)$$

$$\begin{aligned} DD_i = (S\Delta x^2/\Delta t) h\phi_{i,j} - Q_{i,j} + T_{i-1,j} h_{i-1,j} \\ + T_{i,j+1} h_{i,j+1} + Q_a \end{aligned} \quad (11d)$$

For calculations by *rows*, equation 10 is rearranged as follows

$$\begin{aligned} -T_{i-1,j} h_{i-1,j} + h_{i,j} (T_{i-1,j} + T_{i,j} + T_{i,j+1} + T_{i,j-1} \\ + S\Delta x^2/\Delta t) - T_{i,j} h_{i+1,j} = (S\Delta x^2/\Delta t) h\phi_{i,j} - Q_{i,j} \\ + T_{i,j+1} h_{i,j+1} + T_{i,j-1} h_{i,j-1} + Q_a \end{aligned} \quad (12)$$

Equation 12 is of the form

$$AA_i h_{i-1,j} + BB_i h_{i,j} + CC_i h_{i+1,j} = DD_i \quad (12')$$

where the constant terms are

$$AA_i = -T_{i-1,j} \quad (12a)$$

$$BB_i = T_{i-1,j} + T_{i,j} + T_{i,j+1} + T_{i,j-1} + S\Delta x^2/\Delta t \quad (12b)$$

$$CC_i = -T_{i,j} \quad (12c)$$

$$\begin{aligned} DD_i = (S\Delta x^2/\Delta t) h\phi_{i,j} - Q_{i,j} + T_{i-1,j} h_{i-1,j} \\ + T_{i,j+1} h_{i,j+1} + Q_a \end{aligned} \quad (12d)$$

There are three head unknowns in each equation written for each node along a column (equation 11') or row (equation 12'). (In standard matrix notation a set of equations defined by 11' or 12' forms what is termed a tri-diagonal matrix.) The solution of a set of column or row head equations is accomplished by Gauss elimination incorporating what Peaceman and Rachford term G and B arrays applied to tri-diagonal matrices. An explanation of what is included in the G and B arrays follows.

Calculation of Heads with G and B Arrays

An example can be used to illustrate how heads are calculated with the use of the G and B arrays. Although the method outlined can be applied to any number of nodes in a row or column, a four-node row as shown in figure 4 will be considered here, for completeness and simplicity. The heads at the nodes 1, 2, 3, and 4 along the j th row can be calculated by first writing the flow equations (of the form given by equation 12') for each node going in order of increasing column number (i). Secondly, the resulting equations are arranged in such a manner that the head at the node of interest, $h_{i,j}$, is a function of known parameters and the head at only the node $h_{i+1,j}$. When this is done, the head at the last node of the row, $h_{4,j}$, will be a function of known parameters. Finally, all other heads can then be calculated in order of decreasing column number.

The equations for the four nodes shown in figure 4 can be written as follows.

Figure 4. Example four-node row

At the first j th row node, $i = 1$ and the flow equation is (from equation 12')

$$AA_1 h_{1,j} + BB_1 h_{1,j} + CC_1 h_{1,j} = DD_1 \quad (13)$$

Since no node with coordinates $0, j$ exists, AA_1 is set equal to zero and equation 13 becomes

$$BB_1 h_{1,j} + CC_1 h_{1,j} = DD_1 \quad (14)$$

Equation 14 is rearranged into

$$h_{1,j} = DD_1 / BB_1 - (CC_1 / BB_1) h_{1,j} \quad (15)$$

At this point it is defined that

$$\left[\begin{array}{l} G_1 = DD_1 / BB_1 \\ B_1 = CC_1 / BB_1 \end{array} \right] \quad i=1 \quad (16)$$

and

$$\left[\begin{array}{l} G_1 = DD_1 / BB_1 \\ B_1 = CC_1 / BB_1 \end{array} \right] \quad (17)$$

Substituting equations 16 and 17 into 15 gives

$$h_{1,j} = G_1 - B_1 h_{1,j} \quad (18)$$

Now the head at the node of interest $h_{1,j}$ is a function of the known parameters G_1 and B_1 and the head at only the node $h_{2,j}$ or $h_{1,j}$.

Proceeding to the next j th row node of figure 4 where $i = 2$, the equation of flow is written as

$$AA_2 h_{1,j} + BB_2 h_{2,j} + CC_2 h_{2,j} = DD_2 \quad (19)$$

Solving for $BB_2 h_{2,j}$ from equation 19 yields

$$BB_2 h_{2,j} = DD_2 - CC_2 h_{2,j} - AA_2 h_{1,j} \quad (20)$$

Substitution of equation 18 into 20 gives

$$BB_2 h_{2,j} = DD_2 - CC_2 h_{2,j} - AA_2 (G_1 - B_1 h_{1,j}) \quad (21)$$

Carrying out the multiplication, rearranging terms, and solving for $h_{2,j}$ result in

$$h_{2,j} = (DD_2 - AA_2 G_1) / (BB_2 - AA_2 B_1) - [CC_2 / (BB_2 - AA_2 B_1)] h_{1,j} \quad (22)$$

The known parameters of equation 22 are defined as

$$\left[\begin{array}{l} G_2 = (DD_2 - AA_2 G_1) / (BB_2 - AA_2 B_1) \\ B_2 = CC_2 / (BB_2 - AA_2 B_1) \end{array} \right] \quad (23)$$

and

$$B_2 = CC_2 / (BB_2 - AA_2 B_1) \quad (24)$$

Substitution of equations 23 and 24 into 22 gives

$$h_{2,j} = G_2 - B_2 h_{1,j} \quad (25)$$

Again the head of interest $h_{2,j}$ is a function of the known parameters G_2 and B_2 and the head at only the node $h_{3,j}$ or $h_{2,j}$.

Proceeding to the next j th row node where $i = 3$, the flow equation can be written as

$$AA_3 h_{2,j} + BB_3 h_{3,j} + CC_3 h_{3,j} = DD_3 \quad (26)$$

Solving for the terms $BB_3 h_{3,j}$ yields

$$BB_3 h_{3,j} = DD_3 - CC_3 h_{3,j} - AA_3 h_{2,j} \quad (27)$$

Substitution of equation 25 into equation 27 gives

$$BB_3 h_{3,j} = DD_3 - CC_3 h_{3,j} - AA_3 (G_2 - B_2 h_{2,j}) \quad (28)$$

Carrying out the multiplication, rearranging terms, and solving for $h_{3,j}$ result in

$$h_{3,j} = (DD_3 - AA_3 G_2) / (BB_3 - AA_3 B_2) - [CC_3 / (BB_3 - AA_3 B_2)] h_{2,j} \quad (29)$$

The known parameters of equation 29 are defined as

$$G_3 = (DD_3 - AA_3 G_2) / (BB_3 - AA_3 B_2) \quad (30)$$

$$B_3 = CC_3 / (BB_3 - AA_3 B_2) \quad (31)$$

Substitution of equations 30 and 31 into equation 29 yields

$$h_{3,j} = G_3 - B_3 h_{2,j} \quad (32)$$

Finally, the flow equation is written for the last j th row node as

$$AA_4 h_{3,j} + BB_4 h_{4,j} + CC_4 h_{4,j} = DD_4 \quad (33)$$

Since there is no node at $h_{4,j}$ the term CC_4 is set equal to zero and equation 33 becomes

$$AA_4 h_{3,j} + BB_4 h_{4,j} = DD_4 \quad (34)$$

Rearranging terms of equation 34 gives

$$BB_4 h_{4,j} = DD_4 - AA_4 h_{3,j} \quad (35)$$

Substitution of equation 32 into equation 35 gives

$$BB_4 h_{4,j} = DD_4 - AA_4 (G_3 - B_3 h_{3,j}) \quad (36)$$

Carrying out the multiplication, rearranging terms, and solving for $h_{4,j}$ result in

$$h_{4,j} = (DD_4 - AA_4 G_3) / (BB_4 - AA_4 B_3) \quad (37)$$

The head $h_{4,j}$ is a function of only known terms, defined as

$$[G_4 = (DD_4 - AA_4 G_3) / (BB_4 - AA_4 B_3)] \quad (38)$$

Substitution of equation 38 into equation 37 gives

$$h_{4,j} = G_4 \quad (39)$$

Since the head $h_{4,j}$ is now known, substitution of its value back into equation 32 allows calculation of the head at node $h_{3,j}$. The head $h_{3,j}$ is then substituted into equation 32 allowing calculation of $h_{2,j}$. Finally $h_{2,j}$ is substituted into equation 18 giving the value $h_{1,j}$. Thus all heads in the j th row have been determined.

A study of the G and B terms given in equations 16, 17, 23, 24, 30, 31, and 38 reveals their general form as

$$G_N = (DD_N - AA_N G_{N-1}) / (BB_N - AA_N B_{N-1}) \quad (40)$$

and

$$B_N = CC_N / (BB_N - AA_N B_{N-1}) \quad (41)$$

where $N = i$ for row calculations and, by inference, $N = j$ for column calculations. In addition, AA_N is set equal to zero for the first node of a row or column, and CC_N is set equal to zero for the last node of the row or column.

Sets of equations of the form given by equations 40 and 41 for the nodes along a row or column are what Peaceman and Rachford term the G and B arrays. The use of the G and B arrays greatly reduces both the needed computer core storage and execution time.

Examination of equations 18, 25, 32, and 39 reveals the general form for row calculations as

$$h_{i,j} = G_i - B_i h_{i,j+1} \quad (42)$$

Similarly, the general form of the head equations for column calculations is

$$h_{i,j} = G_j - B_j h_{i,j+1} \quad (43)$$

In summary, the process of calculating heads along columns or rows in the digital model includes first computing the values of G and B (equations 40 and 41) for the node of a column or row in order of increasing j or i , respectively. In the course of accomplishing this, the head at the last node of the column or row is found. Equations 42 and 43 are then used to solve for all other heads in the column or row in order of decreasing j or i , respectively. After completing the calculation of heads in an individual column or row, the computer proceeds to the next column or row until all have been processed satisfactorily.