

DECKBLATT


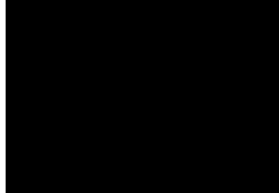
	Projekt	PSP-Element	Obj. Kenn.	Aufgabe	UA	Lfd. Nr.	Rev
	N A A N	N N N N N N N N N N	N N N N N N	X A A X X	A A	N N N N	N N
EU 333	9K	352127.30		EG	EQ	0002	00

Titel der Unterlage: Stellungnahme der GSF zu den Fragen der GRS (lt. Schreiben PTB/18.05.1988) zur Langzeitsicherheits- analyse des Endlagers Konrad: Radionuklidausbreitung in der Nachbetriebsphase (Text und Anlagen A und B)	Seite: I.
	Stand: 07.07.1988

Ersteller: GSF	Textnummer:
--------------------------	--------------------

Stempelfeld:

PSP-Element TP...2.....: 21285	zu Plan-Kapitel: 3.9
--------------------------------	----------------------

	PL 11.07.88  Freigabe für Behörden	PL 11.07.88  Freigabe im Projekt
--	---	--

Diese Unterlage unterliegt samt Inhalt dem Schutz des Urheberrechts sowie der Pflicht zur vertraulichen Behandlung auch bei Beförderung und Vernichtung und darf vom Empfänger nur auftragsbezogen genutzt, vervielfältigt und Dritten zugänglich gemacht werden. Eine andere Verwendung und Weitergabe bedarf der ausdrücklichen Zustimmung.

Revisionsblatt

BfS

EU 333	Projekt	PSP-Element	Obj. Kenn.	Aufgabe	UA	Lfd. Nr.	Rev.
	N A A N	N N N N N N N N N N	N N N N N N	X A A X X	A A	N N N N	N N
	9K	352127.30		EG	EQ	0002	00

Titel der Unterlage: Stellungnahme der GSF zu den Fragen der GRS (Lt. Schreiben PTB/18.05.1988) zur Langzeitsicherheitsanalyse des Endlagers Konrad: Radionuklidausbreitung in der Nachbetriebsphase (Text und Anlagen A und B)	Seite: <div style="text-align: center; padding: 5px;">II.</div>
	Stand: <div style="text-align: center; padding: 5px;">07.07.1988</div>

Rev.	Revisionsst. Datum	verant. Stelle	Gegenzeichn. Name	rev. Seite	Kat. *)	Erläuterung der Revision

*) Kategorie R = redaktionelle Korrektur
 Kategorie V = verdeutlichende Verbesserung
 Kategorie S = substantielle Änderung
 Mindestens bei der Kategorie S müssen Erläuterungen angegeben werden.

Stellungnahme der GSF zu den Fragen der GRS (lt. Schreiben PTB/18.05.1988)
zur Langzeitsicherheitsanalyse des Endlagers Konrad: Radionuklid-
ausbreitung in der Nachbetriebsphase (LV-NR. 2242.03)

A. Rechencode SWIFT

zu 1. und 2.

Die vorliegenden Unterlagen beschreiben die Version BCFT, mit der die Grundwasserberechnungen durchgeführt wurden. Wie in der GSF-Stellungnahme vom 25.11.1987 schon erwähnt, wurde für die anschließende eindimensionale Berechnung des Radionuklidtransports die ältere Version PTCS2 benutzt. In Anlage A sind die Unterschiede in beiden Versionen anhand der vorliegenden Unterlagen beschrieben.

Für die Grundwasserberechnungen in HYDROCOIN wurde die Version BCFT verwendet. Für die Nuklid-
ausbreitungsrechnungen im früheren Projekt INTRACOIN wurden noch ältere Versionen benutzt, die eher der PTCS2-Version entsprechen.

zu 3. und 4.

Wie telephonisch Herr [REDACTED] bereits mitgeteilt, sind die vorgegebenen Druckrandbedingungen an der Oberfläche anders definiert als die gerechneten Drücke an den obersten Blöcken. Daher können sie nicht übereinstimmen. In Anlage B sind die verschiedenen Definitionen der Drücke mit Zustimmung der INTERA zusammengestellt.

Auswerteprogramm STLINE

zu 5. und 6.

Die Dokumentation des neuen Auswerteprogramms SAPT ist in Zusammenhang mit dem Arbeitspaket Grundwasserbewegung nach dem Störzonenmodell KONRAD erstellt worden und liegt als Entwurf bei der PTB vor. Die endgültige Fassung wird GRS von PTB zur Verfügung gestellt. Zur Zeit wird auch die Auswertung der Planrechnungen zum Vergleich mit SAPT durchgeführt.

Eingabeprogramm "POROS"

zu 7. und 8.

Laut unseren Unterlagen entspricht das GRS-Programm "POROS" dem Programm LEIT. Dieses Programm verwendet den Datensatz LEITY (GRS-Bezeichnung "GEO") für Gesteinsarten und ihre Mächtigkeit in jedem Element und berechnet die Durchlässigkeiten für alle Raumrichtungen in jedem Element.

Die steilstehenden Schichten - wie OM im Schnitt $y = 1$ - werden schon im Datensatz LEITY berücksichtigt und kommen im Programm LEIT nicht vor. Eine Dokumentation der Schichtmächtigkeitsangaben in LEITY ("GEO") ist zu aufwendig und nicht unbedingt notwendig. Die Umsetzung der einzelnen steilstehenden Schichten und Unstimmigkeiten können durch Gespräche geklärt werden.



Difference between the two versions of SWIFT-TUB code - BCFT and PTCS2 - as used in the groundwater calculations and radionuclide transport respectively for the long-term safety analysis of the repository KONRAD

Both the versions BCFT and PTCS2 belong to the SWIFT-TUB code family which has been especially installed in TU Berlin by INTERA and enhanced from time to time to incorporate more user comfort and flexibility. In fact the versions BCFT and PTCS2 were two of the latest enhancements in TUB, of which BCFT is the most current version. The version BCFT includes the following extensions as compared to PTCS2:

1. Permission of decoupling boundary conditions for pressure, temperature and concentration.
2. Pressure values for boundary conditions (aquifer influence functions) are calculated internally if hydrostatic pressure distribution is desired.
3. Inclusion of the effect of free water surface, also referred to as water table conditions.
4. Permission to use recharge in m/sec in the uppermost layer.
5. An additional restart option with initial values for P, T and C saved in a previous run is available.

The users' manual of BCFT-version is available. It should thus be changed by deletion of parameters as shown in the enclosure to obtain the corresponding documentation for the PTCS2-version. The changes have been marked with numbers indicating the omission of the above mentioned extensions.

6.1.1 The "M" and RO" Cards

The "M" cards are read from the main program. The information provided by these cards sets up a general framework which the analysis will build on. The framework includes items such as:

Which equations will be solved,
The type of wellbore calculations to be used,
Setting printing and plotting controls,
Grid size,
Type of aquifer representation,
The method of numerical solution to be used.

The "RO" cards input information pertaining to the radioactive components. This information defines each isotope in terms of its parents; branching ratios for each parent, mass of the isotope, half life and distribution coefficient for each rock type.

Read M-1 (20A4/20A4) Title.

LIST: TITLE

TITLE Two cards of alphanumeric data to serve as a title for this run. Any title up to 160 characters (80/card) in length may be used.

READ M-2 (7I5) Option Parameters.

(3) LIST: NCALL, RSTRT, ISURF, IIPRT, NPLP, NPLT, NPLC, IUNIT

NCALL Control parameter for solving the basic partial differential equations. To solve all three equations, enter zero.

(3)

IIPRT	Transmissibility printing key. The value entered here is not used. This version of the model has been modified to read IIPRT in READ R2-13 which activates printing of several intermediate parameters on a one time step basis.
-------	--

NPLP Control parameter for plotting pressures in the wells.

- 1 - Bottom-hole and surface pressures are plotted if wellbore calculations are performed. Only the bottom-hole pressures are plotted if no wellbore calculations are performed. For an observation well the bottom-hole pressure is the grid block pressure.
- 0 - No pressure plots are desired.
- 1 - Pressure plots are desired for a previous run. Skip READ M-3 through R2-18 and proceed to Read P-1.

NPLT Control parameter for plotting temperatures in the well.

- 1 - For an observation well the grid-block temperature is plotted. For an injection well the bottom-hole temperature is plotted if wellbore calculations are performed. For a production well the bottomhole temperature is always plotted. In addition the surface temperature is plotted if the wellbore calculations are performed.
- 0 - No temperature plots are desired.
- 1 - Temperature plots are desired for a previous run. Skip READ M-3 through R2-18 and proceed to READ P-1.

NPLC Control parameter for plotting concentration in the well.

- 1 - The concentration in the well is plotted for observation and production wells only.
- 0 - No concentration plots are desired.
- 1 - Concentration plots are desired for a previous run. Skip READ M-3 through R2-18 and proceed to READ P-1.

IUNIT Unit specification control.

0 - SI System

1 - English Engineering System

NOTE: Proceed to READ P-1 if any of NPL's are negative.

NOTE: Skip to READ M-4 if this is a restart run, i.e., RSTRT > 0.

READ M-3 (List 1: 8I5, List 2: 8I5) Core Allocation and Control.

LIST 1: NX, NY, NZ, HTG, NCP, NRT, KOUT, PRT

(4) LIST 2: NSMAX, NABLMX, NRCHMX, METHOD, NAAR, NTIME, NCOMP, NREPB

ERROR MESSAGE:

(Number 1) NX is less than or equal to one or
NY is less than one or
NZ is less than one.
The minimum dimensions on the grid block system are
2x1x1. The maximum size is limited only by the
available computer storage.

(Number 7) HTG is not within the permissible range.
HTG is less than 1 or greater than 3.

(Number 8) The entered value for KOUT is not permissible. KOUT
is not equal to 0, 1 or 3.

(Number 9) PRT exceeds permissible range of -1 to +2.

NX Number of grid cells in the x direction (greater
than or equal to 2).

NY Number of grid cells in the y direction (greater
than or equal to 1).

NZ Number of grid cells in the z direction (greater
than or equal to 1).

HTG Control parameter for input of reservoir descrip-
tion data.

1 - Homogeneous aquifer, cartesian geometry.

2 - Heterogeneous aquifer, aquifer data entered
on regional basis, cartesian geometry.

3 - Radial geometry. The aquifer may be heter-
ogeneous in the vertical direction.

NCP Number of radioactive/trace components in the
system.

NRT Number of rock types.

NOTE: Distribution coefficients, dispersivities, thermal conductivities and salt-dissolution coefficients are all functions of rock or strata type. Rock types of all blocks are initialized to IRT = 1. Changes of rock type to other values are entered in the RIA-1 cards.

KOUT Output control.

0 - All initialization output activated.

1 - All initialization output except initial arrays (concentrations, pressures, etc.) are activated.

3 - No initialization output is activated. A value of 3 for KOUT can be used to omit printing of most initialization data.

PRT Output array orientation control.

-1 - Print output arrays as areal layers (x-y). Block numbers in the x direction increase from left to right and decrease down the computer page in the y direction.

+1 - Printout is similar to above except that J-block numbers increase down the computer page.

2 - Print output arrays as vertical sections (x-z).

NSMAX Maximum number of radioactive/trace component sources that will be used during the run.

NABLMX Maximum number of aquifer influence function blocks. This data is used for dimensioning the aquifer influence function arrays. This number is equal to the number of peripheral blocks, if aquifer influence functions are to be used.

(4)

NRCHMX Maximum number of surface recharge blocks

NOTE: The read group consists of two cards or any number of sets of two cards, each set defining a rectangular region and the value of VAB to be assigned that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read to be assigned to the overlapped subregion. If these data are read, i.e., IAQ ≠ 3, then skip READS R1-29 through R1-32 and proceed to READ R1-33.

LIST 1: I1, I2, J1, J2, K1, K2, KAQ, IPTC

LIST 2: VAB, P1, T1, C1, T2, T3, C2

ERROR MESSAGE:

(Number 18)

IAQ is greater than 4, or one or more of I1, I2, J1, J2, K1, K2, are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.

I1, I2 Lower and upper limits, inclusive, on the I-coordinate of the aquifer influx region.

J1, J2 (Similar definition for J-coordinate).

K1, K2 (Similar definition for K-coordinate),

KAQ Control variable for heat-transport equation only for IAQ = 4.

-1 - Type 3 radiation condition only. T1 is not used. T2 and T3 are used.

0 - Type 1 temperature condition only. T1 is used. T2 and T3 are not used.

1 - Type 1 temperature condition and Type 3 radiation condition. T1, T2, and T3 are all used.

Three digit number to specify the boundary conditions for P, T, C (radionuclide and inert component), decoupling of P, T, C is possible

IPTC = 000, boundary is open for P, T and C; transport by convection, diffusion and dispersion

= 110, boundary is closed for P and T; transport by diffusion and dispersion only

= 011, boundary open for convective flow only, no diffusive and convective transport for heat and salt

(4)

For IAQ = 1 or 2 (READ R1-27)

VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft^3/psi (m^3/Pa) for a pot-aquifer representation and $\text{ft}^3/\text{psi-day}$ ($\text{m}^3/\text{Pa-sec}$) for a steady-state representation.

P1, T1, C1, T2, T3 Not used.

For IAQ = 4 (READ R1-27)

VAB Boundary block type.

- 1.0 - Block is located on an I = 1 edge.
- 2.0 - Block is located on an I = NX edge.
- 3.0 - J = 1 edge.
- 4.0 - J = NY edge.
- 5.0 - K = 1 edge.
- 6.0 - K = NZ edge.

P1, T1, C1 Constant values of pressure in psi (Pa), temperature in °F (°C) and concentration (fraction) at the block boundary specified according to VAB and KAQ.

(2)

~~For VAB = 1, 2, 3, and 4, constant values of pressure are to specify only for K = 1. Pressure values for K > 1 are calculated internally using a hydrostatic pressure distribution. P(K = 1) must be ≠ 0.~~

T2 Temperature of surrounding media, °F (°C).

T3 Coefficient of surface heat transfer $\text{Btu/day-ft}^2\text{-}^\circ\text{F}$ ($\text{W/m}^2\text{-}^\circ\text{C}$).

C2 Brine and radionuclide mass transfer coefficient at block boundary (transmissibility), $\text{kg/m}^2\text{-s}$. If C2 = 0 transmissibility will be calculated for boundary internally.

NOTE: If IAQ is not equal to 3, omit these data and proceed to READ R1-33. This section is used to enter data for the Carter-Tracy method of calculating aquifer influence functions.

6.1.3 The "I" Cards

These data are read for initializing concentrations and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer and there is no natural flow, insert a blank card and proceed to READ R1A-1.

READ I-1 (4I5) Initial Velocity and Concentrations.

NOTE: The first three data are read for initializing concentrations and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer and there is no natural flow, insert a blank card and proceed to READ R1A-1. The fourth value is to initialize from a tape.

LIST: ICOMP, INAT, IRD, ~~IRST~~

- ICOMP Control parameter for initializing brine concentrations.
- 0 - Initial concentrations in all the grid blocks are zero.
 - 1 - The initial brine concentrations are not zero everywhere. Nonzero concentrations will be entered in READ I-2.
- INAT Control parameter for entering initial fluid velocity.
- 0 - The aquifer fluid is static initially.
 - 1 - The resident fluid velocity will be entered in READ I-3.
- IRD Control parameter for initializing radioactive/trace component concentrations.
- 0 - Initial concentrations in all the grid blocks are zero.
 - 1 - Nonzero concentrations for each component will be entered in READ I-4.

(5)

~~IRST Option for initializing with calculated values from a previous run. To initialize temperature/concentrations the saved values of the pressure distribution is needed too.~~

- ~~0 - No initializing~~
- ~~m > 0 - Initializing with values from a previous run~~
 - ~~m = 100 pressure distribution~~
 - ~~= 110 pressure and temperature distribution~~
 - ~~= 101 pressure and brine distribution~~
 - ~~= 111 pressure, temperature and brine distribution~~

NOTE: The user should enter NCOMP groups of cards as specified in READ R1A-8. However, the information will be used only in those cases where CNAME matches DI, as specified in READ R0-1.

READ R1A-8 (2A4, 2X, 7E10.0,/(8E10.0)) Interpolation of Repository Concentrations.

LIST: (CNAME(I), I = 1,2), (CNDUM(I), I = 1, NTIME)

CNAME	Identification of radioactive component
CNDUM	If interpolation is to be used, then CNDUM represents the concentrations at the interpolation times expressed as mass per unit volume of waste. If interpolation is not used, then CNDUM(1) is the initial concentration.

READ R1A-9 (7F10.0) Solubility Limits.

LIST: (CS(I), I = 1, NCP)

ERROR MESSAGE:

(Number 61) One or more of the solubilities is negative.

CS	Solubility limits expressed as mass fractions.
----	--

6.1.5 The "R2" Cards (Recurrent Data)

The data defined in the previous section are required to describe the aquifer and fluid properties and to establish initial conditions. The data discussed in this section, however, are time-dependent. They are read before the first time step and at subsequent time steps when changes are desired in the time-step data, the wells, the source data, the wellbore data, the solution method, or the mapping specifications. Note that any of the data entered up to this point cannot be changed. The overburden and underburden blocks specifications or aquifer influence functions cannot be changed in any manner once they have been specified at the beginning.

READ R2-1 (10I5) Control Parameters.

(4) LIST: INDQ, IWELL, IMETH, ITHRU, IRSS, IPROD, IOPT, INDT, ICLL, IRCH

INDQ	Control parameter for reading well rates.
0	- Do not read well rates.
1	- Read well rates on one card (READ R2-5).
2	- Read one card for each well rate (READ R2-6).

INDT Control parameter for reading reservoir solution iteration data for the reservoir solution.

0 - Do not read iteration data. If entering data before the first time step, default values of the iteration parameters will be used.

1 - Read new or altered iteration data.

ICLL 0 - Do not read change in equation solution control, NCALL

1 - Read new equation solution control, NCALL.

IRCH 0 - No change in recharge data.

1 - Recharge data will be initialized or updated during this time step.

(4)

(4) READ R2-2.5 (4I5,E10.0) Recharge Data

NOTE: Skip this READ, if IRCH = 0. For overlapping blocks, the rate read latest will be used. Follow the last card with a blank card.

LIST: I1, I2, J1, J2, RCHG

I1, I2	Recharge blocks in the X-direction
J1, J2	Recharge blocks in the Y-direction
RCHG	Recharge rate in the uppermost layer (k = 1) [m/sec]

READ R2-3 (I5, 4F10.0) Wellbore Data.

NOTE: These data are entered if IOPT is greater than zero. If default values are desired, insert a blank card and proceed to READ R2-4. The default values of the parameters are discussed below.

LIST: NITQ, TOLX, TOLDP, DAMPX, EPS

NITQ	Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the wellhead pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If entered as zero or a negative number, the program selects the default value of 20.
TOLX	The tolerance on the fractional change in pressure over an iteration. If entered as zero or a negative number, the default value of 0.001 is selected.
TOLDP	The tolerance, on pressure, psi (Pa). The default value is 7000 psi (4.8×10^7 Pa).
DAMPX	Damping factor in estimating the next value of the pressure (surface for an injection well and bottom-hole for a production well). If the frictional pressure drop in the well is high, a linear extrapolation may lead to oscillations around the right value. The default value is 2.0.
EPS	The tolerance on calculating temperature from given values of enthalpy and pressure. The fluid temperatures in the wellbore are calculated over each pressure increment as specified in READ R1-3. The default value is 0.001.

ISAVEP, ISAVET, 0 - no save up to TCHG inclusive
 ISAVEC, ISVCRN n > 0 - save at every n-th time step and
 at TCHG on tape 9
 < 0 - save only at TCHG on tape 9

(5)

and for -2 - additional saving at TCHG on tape 11
 with ISAVEP referring to PDAT
 ISAVET referring to T
 ISAVEC referring to C (brine)
 ISVCRN referring to CRN

 READ R2-13.6 (List 1: I5, List 2:3I5)

NOTE: Skip this READ, if ISVBL = 0

LIST 1: NBLS

LIST 2: ISVCBL (IBLS), JSVCBL (IBLS), KVCBL (IBLS)

IBLS = 1,..NBLS

NBLS Number of grid blocks for which concentration
 are to be saved.

NBLS = 0 no save up to TCHG inclusive

ISVCBL (IBLS), JSVCBL (IBLS), KVCBL (IBLS): Location of
 block IBLS.

 READ R2-14 (I5, 2F10.0) Map Data.

NOTE: Enter these data only if contour maps are desired (MAP is
 not equal to 0000), and if MDAT is equal to one.

LIST: NORIEN, XLGTH, YLGTH

NORIEN Map orientation factor.

0 - The map is oriented with x (refers to r for
 radial geometry) increasing from left to
 right and y (z for radial geometry or for
 cartesian geometry with NY = 1) increasing
 up the computer page, i.e. the x = 0, y = 0
 point is the lower left-hand corner.

1 - The map is oriented with x increasing from
 left to right and y (z for radial geometry or
 for cartesian geometry with NY = 1)
 increasing down the computer page. The
 origin is the upper lefthand corner.

XLGTH The length, in inches, on the computer output
 which is desired in the x (or r) direction.

YLGTH The length, in inches, on the computer output
 which is desired in the y (or z for radial geo-
 metry) direction.

GSF/Ift/ENS
Gruppe Sicherheitsanalyse

Braunschweig, July 7th, 1988
[REDACTED]/0.165

Pressure definition in SWIFT-TUB code

The definitions of different fluid pressures (pressure at elevation or absolute pressure and pressure at datum or dynamic pressure) as they are put as initial and boundary conditions or calculated as results of the SWIFT-code have not been provided clearly in any documentation. The different versions of commercially available SWIFT code use even different locations in the block for these definitions. In this note the pressure definitions as used in the SWIFT-TUB code have been documented with written approval from INTERA.

M E M O

TO :



FROM:



CC :

DATE: 5TH JULY 1988

RE: PRESSURE DEFINITION IN SWIFT-TUB

Absolute fluid pressure is depth/height dependent. No-flow conditions are described by a hydrostatic pressure gradient. Flow gradient is deviation from the hydrostatic pressure gradient.

$$u = \frac{k}{\mu} (\rho - fgh)$$

The quantity $(p - fgh)$ is the deviation from the hydrostatic ^{pressure} gradient, known as the dynamic pressure.

All the depths and pressures in SWIFT-TUB are defined at the top of the grid blocks. The reason for this is that generally geologic structure maps are defined at the top of the formations. The finite-difference equations are being solved for block averaged pressure, temperature and concentration values. Therefore all the pressure values used in SWIFT are average values (or approximated to grid center values) adjusted to top of the block.

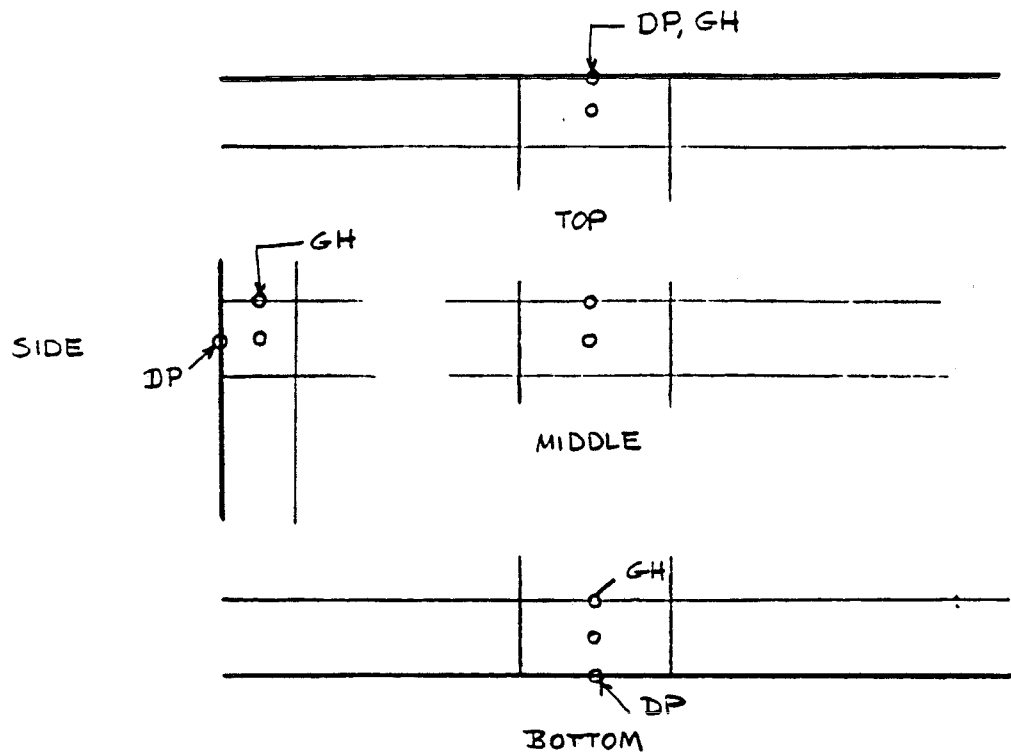
I believe the explanations stated in your fax accurately represent the pressure definitions.



.....

LOCATION OF PRESSURE BOUNDARY CONDITIONS AND PRESSURE OUTPUTS FOR DIFFERENT BLOCKS IN SWIFT-TUB

1. PRESSURE BOUNDARY CONDITIONS

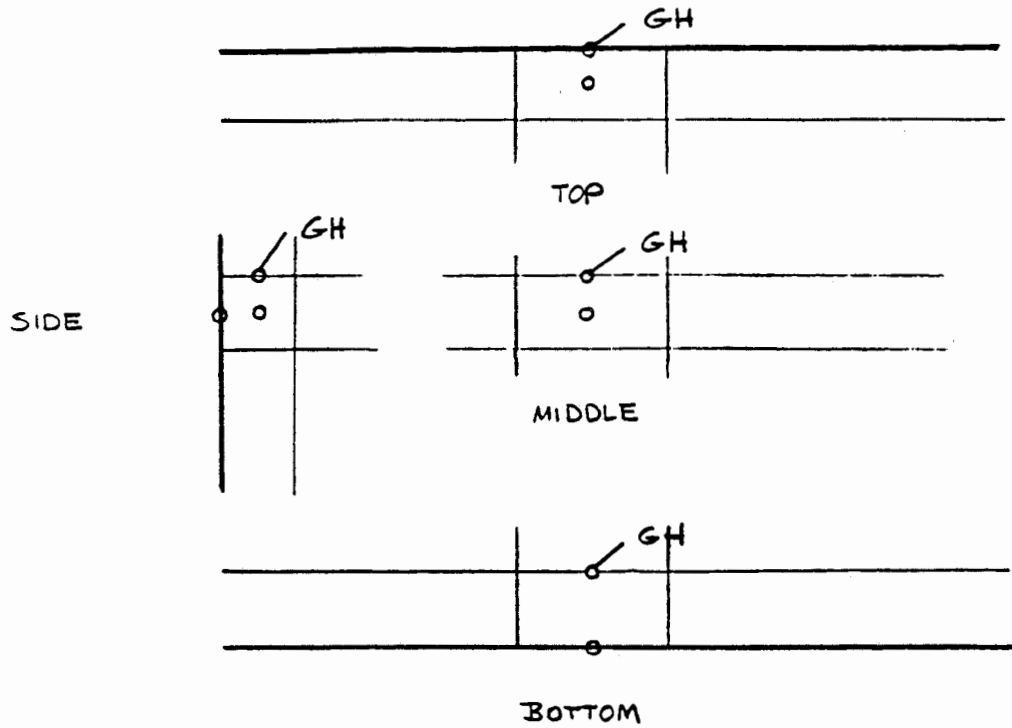


Constant boundary pressure at the top, bottom and side block

--> dynamic pressure (DP) +
pressure corresponding to the geodatic height (GH)

LOCATION OF PRESSURE BOUNDARY CONDITIONS AND PRESSURE OUTPUTS FOR DIFFERENT BLOCKS IN SWIFT-TUB

2. INITIAL PRESSURE



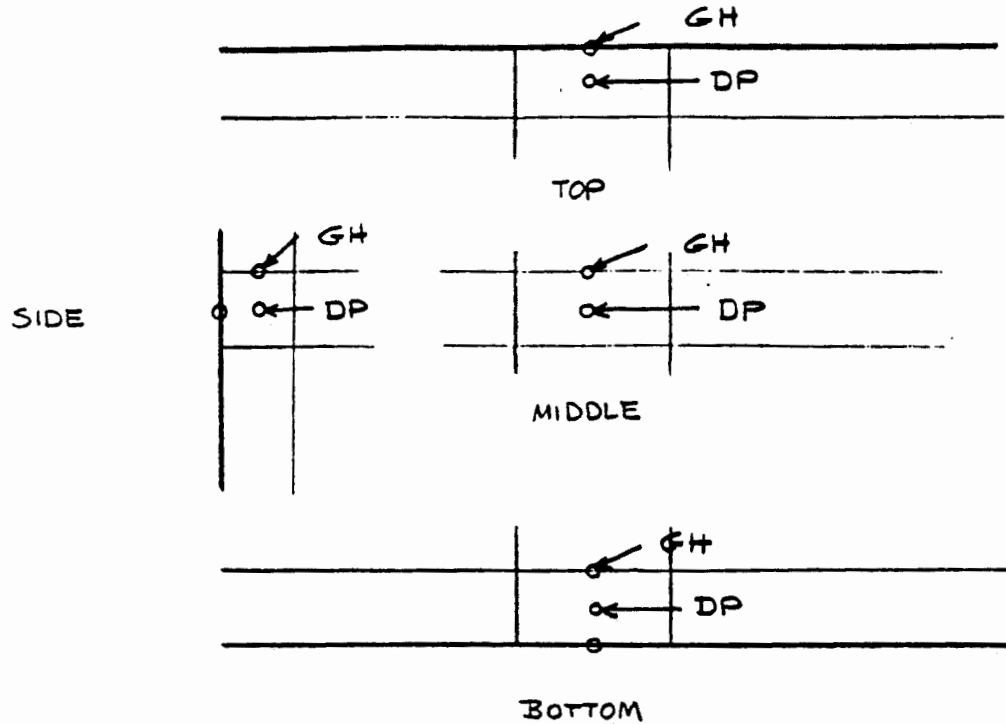
Initial pressure at any block

--> hydrostatic pressure

corresponding to the geodatic height (GH)

LOCATION OF PRESSURE BOUNDARY CONDITIONS AND PRESSURE OUTPUTS FOR DIFFERENT BLOCKS IN SWIFT-TUB

3. CALCULATED PRESSURE



Calculated pressure at elevation H

- > dynamic pressure (DP) +
pressure corresponding to the geodetic height (GH)

Calculated pressure at datum

- > dynamic pressure (DP)
- > pressure at elevation H -
pressure corresponding to the geodetic height (GH)