

User guide for leaky-unconfined code

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1 Input

Each of the options used in the `input.dat` file are explained here. There are comments listed to the right of the options, typically preceded by “::” (but this isn’t required). The entries can be entered in “free” format using decimal or exponential notation with spaces or tabs between the entries. Everything after the last numerical entry on each line is ignored by the program, and therefore consists of comments describing the entries.

The first line of the input file is comprised of logical (T or F) options. Valid inputs are T, True, .true., F, False, and .false..

::old coord system?, general leak-unconf soln?, piezometer?, Neuman72?, Neuman74?, Hantush64?, classical?, compute lambda?, slimy?

1. `old coord system?` The 2007 paper [Malama et al., 2007] and the 2008 paper [Malama et al., 2008] use different coordinate conventions (see Figure 1). For the two-layer system, the coordinate origin is at the bottom of the pumping well (z positive up into the aquifer, negative down into the aquitard), while for the three-layer system the coordinate origin is where the pumping well intersects the land surface. The values used in the rest of the program have different meaning, depending on which system is being used.
2. `general leak-unconf soln?` T indicates the solution from either the 2007 or 2008 paper will be computed (generally what you want).
3. `piezometer?` T indicates the observation location is a point (no z dimension), otherwise the observation well has a screen top and bottom.
4. `Neuman72?` T indicates the unconfined (but non-leaky) solution of Neuman [1972] will be computed at the same times and locations for comparison.
5. `Neuman74?` T indicates the partially-penetrating unconfined (but non-leaky) solution of Neuman [1974] will be computed at the same times and locations for comparison.
6. `Hantush64?` T indicates the partially-penetrating confined (not unconfined or leaky) solution of Hantush [1964] will be computed at the same times and locations for comparison.
7. `classical?` T indicates an unpublished “classical” leaky-unconfined solution, with leaky behavior analogous to Hantush and Jacob [1955], will be computed at the same times and locations. This uses the geometry convention of the 2007 paper.

8. `compute lambda`? T indicates that the parameter λ (in the classical solution) will be computed from the specified aquifer and aquitard parameters, otherwise it can be specified directly.
9. `slimy`? If there are problems getting the solution to produce valid results at very small and very large times, this may “help”, since it essentially throws out any errors, rather than returning “NaN” or “infinity” as it should. It is better not to use this (leave as F).

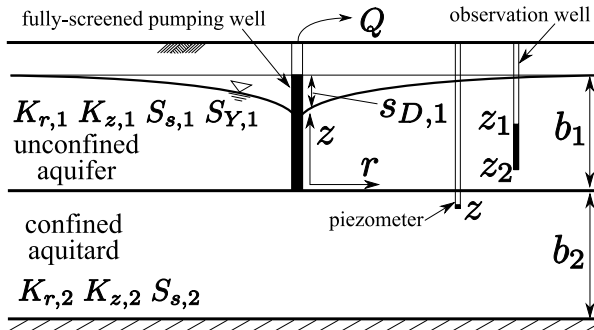


Figure 1 from Malama et al. [2007]

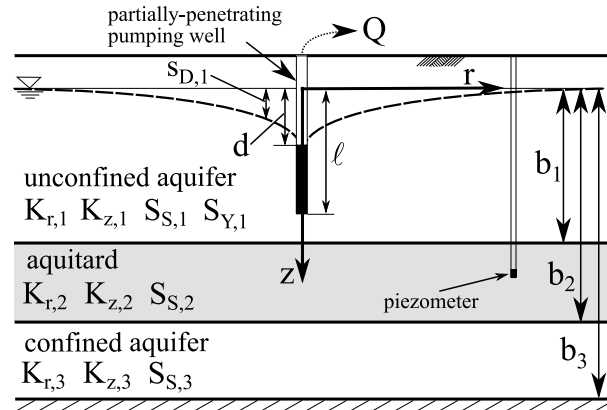


Figure 1 from Malama et al. [2008]

The next few lines of the input file specify most of the geometry and aquifer/aquitard parameters.

```
:: top of pumping well screen(dd), bottom(ld)
:: layer thicknesses, lambda (only used if compute lambda above is false)
:: unconfined upper aquifer Kr, Kz
:: aquitard Kr, Kz
:: confined lower aquifer Kr, Kz
:: Ss1,Ss2,Ss3
:: upper aquifer Sy
```

1. `top/bottom of pumping well screen` If the 2008 solution is being used, these specify the dimensionless top (d_D) and bottom (l_D) of the pumping well screen. If the 2007 solution is selected, these are not used.
2. `layer thicknesses, lambda` If using the 2007 solution, only the first two numbers are read: actual thickness of layer 1 (aquifer) and layer 2 (aquitard). For the 2008 solution these values are layer 1 (unconfined aquifer), layer 2 (aquitard), and layer 3 (confined aquifer) – see Figure 1. Lambda is only used in the “classical” solution.
3. `unconfined upper aquifer Kr, Kz` The radial ($K_{r,1}$) and vertical ($K_{z,1}$) hydraulic conductivities for the pumped aquifer.
4. `aquitard Kr, Kz` The radial ($K_{r,2}$) and vertical ($K_{z,2}$) hydraulic conductivities for the aquitard.
5. `confined lower aquifer Kr, Kz` The radial ($K_{r,3}$) and vertical ($K_{z,3}$) hydraulic conductivities for the unpumped aquifer (not used in 2007 solution, but required as a placeholder).

6. **Ss1, Ss2, Ss3** The specific storages for the three layers, $S_{s,1}$, $S_{s,2}$, and $S_{s,3}$.
7. **upper aquifer Sy** The specific yield for the pumped aquifer, S_y .

The next few lines specify solution options and some geometry

```
:: number of times to solve
:: obs loc: zD, rD, ztop & zbot, Gauss Quad order for screened well
:: invlap alpha (largest pole), invlap tolerance, number FS terms (2M+1)
:: H-1epsabs, epsrel, maxsub, min/max split at, #zeros to integrate , order of G-Lquad
```

1. **number of times to solve** a few lines later in the input file, at least this many times must be listed.
2. **obs loc: zD, rD, ztop & zbot, Gauss Quad order for screened well** These parameters are related to the observation well.
 - z_D is the dimensionless z coordinate for a piezometer (note the different convention in 2007 and 2008 papers).
 - r_D is the dimensionless radial distance from the pumping well to the observation point/well.
 - z_{top} and z_{bot} are the top and bottom of the observation well (only used if the “piezometer” variable in the first line is false), these also have different convention, based on whether the 2007 or 2008 solution is selected.
 - **Gauss Quad order for screened well** is the order of Gauss quadrature used to integrate the solution over the well screen. Valid orders are 1–10,12, and 20.
3. **invlap alpha (largest pole), invlap tolerance, number FS terms (2M+1)** These parameters are related to the inverse Laplace transform algorithm of de Hoog et al. [1982].
 - **invlap alpha (largest pole)** This is a non-negative real number, close to zero. For the application use here 1.0×10^{-14} is usually a good value.
 - **invlap tolerance** This is a non-negative real number related to the desired tolerance in the computed solution. It must be $> \alpha$.
 - **number FS terms (2M+1)** This is an integer (M), indicating the number of Fourier series terms to utilize in the expansion. More terms generally leads to a more accurate solution, but more effort is required to compute it. *At very small and very large times, a large M can lead to un-necessary numerical overflow.* $10 \leq M \leq 20$ is generally a good range.
4. **H-1epsabs, epsrel, maxsub, min/max split at, #zeros to integrate, order of G-Lquad** These parameters are related to the numerical inverse Hankel transform, as described in Malama et al. [2008], and illustrated in Figure 1.
 - $\mathcal{H}^{-1}\epsilon_{\text{abs}}$ is a positive real number, the absolute error desired in the QXGS integration routine [Favati et al., 1991], used for the finite portion of the Hankel integral.
 - $\mathcal{H}^{-1}\epsilon_{\text{rel}}$ is a positive real number, the relative error desired in the QXGS integration routine.
 - **maxsub** is an integer, the maximum number of abscissa to compute in the QXGS automatic quadrature routine

- `min/max split` are two integers, indicating the minimum and maximum number of the zero of the Bessel function (n in $j_{0,n}$) to split between the finite integral (handled using QXGS) and the infinite integral (handled using accelerated Gauss-Lobatto quadrature). The minimum split \leq maximum split, and they both must be ≥ 1 . At small radial distances, the split is made as large as possible, and at large radial distances it is made as small as possible. Making these both 1 or 2 is actually ok.
- `#zeros to integrate` is an integer, indicating how many zeros should be integrated to give a series of areas that are then accelerated using Wynn's ϵ algorithm Wynn [1966] to approximate the infinite portion of the integral. A larger number accelerates a larger series, which should lead to more accurate results, but the integral can \rightarrow "NaN" if this is made too large. A minimum number of terms (5) is required to produce useful results.
- `order of G-Lquad` is an integer indicating the order of the Gauss-Lobatto quadrature used to integrate between the zeros of the J Bessel function. Valid orders are 5–12.

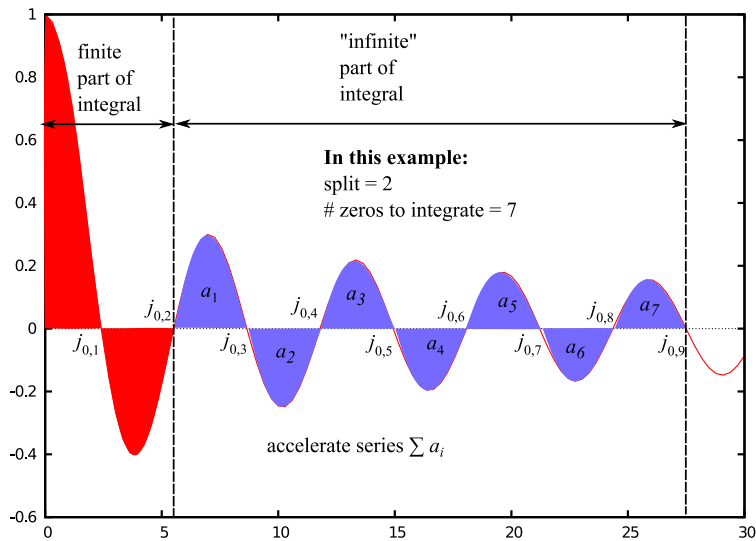


Figure 1: numerical Hankel inversion illustrated for $J_0(r) \times 1$

The last two lines have the times to compute the solution and the filename desired for the output. The times should be put all in one row (they can be computed in a spreadsheet and pasted into the input file).

2 Output

The output generated by the program is briefly described. All the input parameters are echoed to the output file, for both debugging and keeping track of which parameters were used to generate which output. All lines beginning with “#” are “comments”.

The output will be in columns, with the dimensionless time (t_D) as the first column, and the solutions as the subsequent columns. There are two blank lines and another section of data, listing the solutions that were computed for comparison (e.g., Neuman 1972, Neuman 1974, Hantush 1964, Theis, etc.).

The output is formatted for plotting with Gnuplot (<http://www.gnuplot.info>), but other plotting programs should be able to use this format as well.

References

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