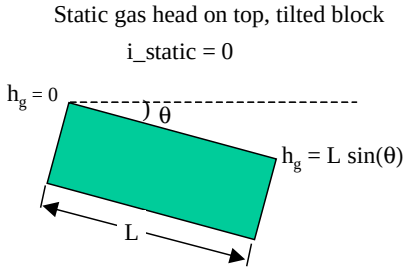
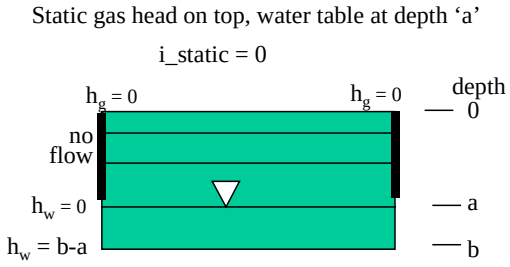
2D version

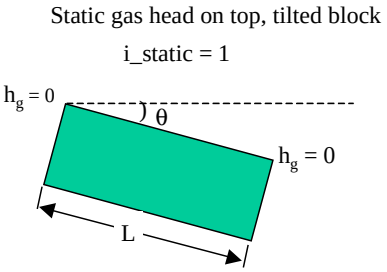
The following changes are discussed below: 1.) new compiler switch, 2.) new iterative matrix solver, 3.) direct solver compiler option has been removed, 4.) graphics output file structure has changed to support GMS, 5.) errors in the code fixed, and 6.) modified 3-phase k-S model incorporated.

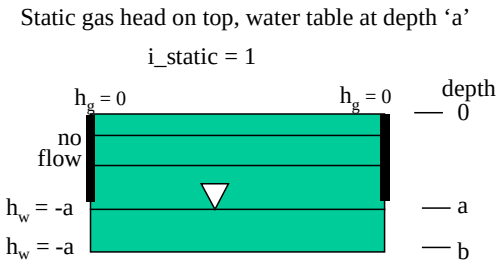
1.) New compiler switch. In file 'include.f' the parameter 'i_static' has been added. This affects how flow boundary conditions are specified, specifically, pressure head. i_static can take on two values, 0 or 1. If = 0 then, if phase head is to be defined at a node, the total head is prescribed (note, this is the scheme described in the documentation). The figures below provide examples.





If i_phase = 1, then if phase head is to be defined at a node, only the difference from static head is prescribed. The figures below provide examples.





This option is intended to make specifying flow BCs easier, especially in the tilted grid case.

2.) New iterative matrix solver. A bi-Conjugate gradient algorithm with an ILU pre-conditioner has replaced the GMRES solver. This solver is more efficient than the GMRES algorithm both in terms of memory and convergence. With the biCG there is no need to specify 'nsave,' and this parameter has been removed as a compiler switch from the **include.f** file.

3.) The direct solver option and related subroutines have been removed. The compiler switches in file **include.f**, *itsol_f* and *itsol_t* have been removed. All matrix problems are solved using the bi-CG iterative solver.

4.) OUTPUT The graphics output option is now set up to be compatible with GMS. All is the same as described in the documentation for input line 17 (page 120), except now the post-processor is GMS, the grid is defined in file **grid.2dg**, and the output files have extension 'dat'.

5.) Two bugs have been removed. One in file satpar.for and one in pe_co.for.

6.) The k-S functionals have been altered as follows:

Relative Permeability of water:

$$k_{rW} = (S_{eW})^{\zeta}\left\{\left[1-(S_{We})^{1/m}\right]^{m} - \left[1-(S_{W})^{1/m}\right]^{m}\right\}$$

where,

$$S_{eW} = (S_W - S_{We}) / (1 - S_{We} - S_{Ne} - S_{Ge})$$

and all terms are defined in Section 5.3 of the manual.

Relative Permeability of gas:

$$k_{rG} = (S_{eG})^{p}\left\{\left[1-(1-S_G)^{1/m}\right]^{m} - \left[1-(1-S_{Ge})^{1/m}\right]^{m}\right\}$$

where,

$$S_{eG} = (S_G - S_{Ge}) / (1 - S_{We} - S_{Ne} - S_{Ge})$$

and all terms are defined in Section 5.3 of the manual.

Relative Permeability of NAPL:

$$k_{rN} = (S_{eN})^{\xi}\left\{\left[1-\left(S_W + S_{Nwt}\right)^{1/m}\right]^{m} - \left[1-\left(1-S_G - S_{Nat}\right)^{1/m}\right]^{m}\right\}$$

where,

$$S_{eN} = \left(S_N - S_{Nt}\right)/\left(1 - S_{Wt} - S_{Nt} - S_{Gt}\right)$$

and $S_{Nnt} + S_{Nwt} = S_{Nt}$ where, S_{Nwt} is that part of total NAPL entrapment (S_{Nt}) that is entrapped as a wetting phase, and S_{Nnt} is that part of S_{Nt} that is entrapped as a non-wetting phase. The differentiation is approximated herein as:

$$S_{Nwt} = S_{Nt}\left(\frac{S_G}{S_W + S_G}\right); \quad S_{Nat} = S_{Nt}\left(\frac{S_W}{S_W + S_G}\right)$$

All other terms are defined in Section 5.3 of the manual.

Currently, these definitions for the k-S functionals are fixed. Therefore, the only 'fitting' parameters for he k-S model are the pore connectivity parameters, $\zeta, \varphi,$ and ξ (input parameters *alfw*, *alfn*, and *alfg* on lines 41, 42 and 43 of the input file **sm.in**, respectively). Note, input parameters *nesw1* and *nesw2* on line 41, *nesn1, nesn2* and *nesn3* on line 42, and *nesg1* and *nesg2* on line 43 are currently ignored by the simulator.

3-D version.

There are several changes. The first two changes are aimed at making the code more memory efficient. The third is aimed at making flow boundary condition input easier. The forth has to do with graphics output. The fifth describes a modification of the k-S model. The sixth describes bug fixes.

1.) As with the 2D version a new iterative matrix solver is now used. It is a bi-Conjugate gradient algorithm with an ILU pre-conditioner. This solver is more efficient than the GMRES algorithm both in terms of memory and convergence. With the biCG there is no need to specify 'nsave' and this parameter has been removed.

2.) New compiler switch. If species transport is not being used, option to eliminate memory requirements for related parameters. For example, if only modeling multiphase flow, then set the parameters i_ow = 0 and i_og = 0 (see the file 'include.f'). If you just want to model water-phase species transport then set the parameters i_ow = 1 and i_og = 0. If you just want to model water- and gas-phase species transport then set the parameters i_ow = 1 and i_og = 1. An error message is issued if there is an incompatibility.

3.) As with the 2D version the compiler parameter i_static is implemented (see file 'include.f'). If i_static = 1, then specify the difference from static head conditions. Included to simplify BC input.

4.) OUTPUT. The graphics output option is now set up to be compatible with GMS. All is the same as described in the documentation for input line 17 (page 120), except now the post-processor is GMS, the grid is defined in file **grid.3dg**, and the output files have extension 'dat'.

5.) The k-S model has been altered as described for the 2D version, part (6).

6.) As with the 2D version, two bugs have been removed. One in file satpar.for and one in pe_co.for.