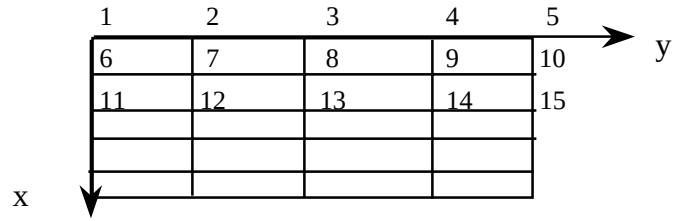
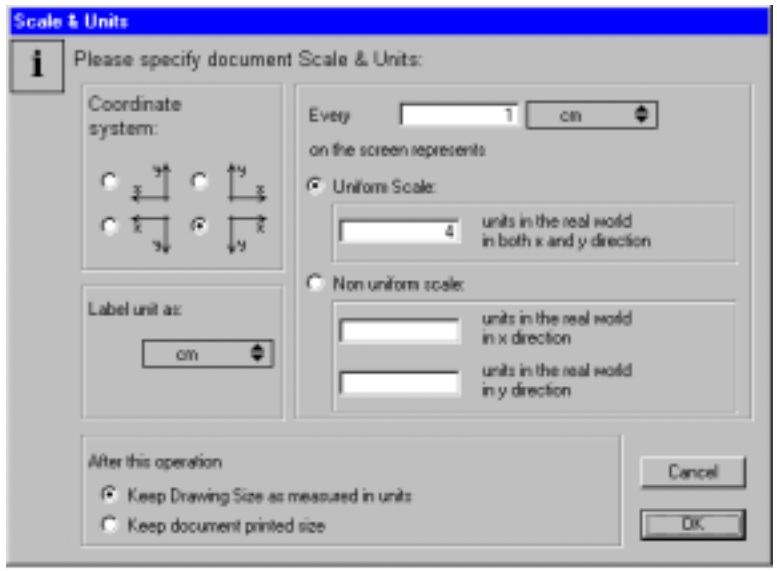
THE SETUP get oriented
get the code ready to run

Default axis orientation
and node numbering



Setup in ArgusONE



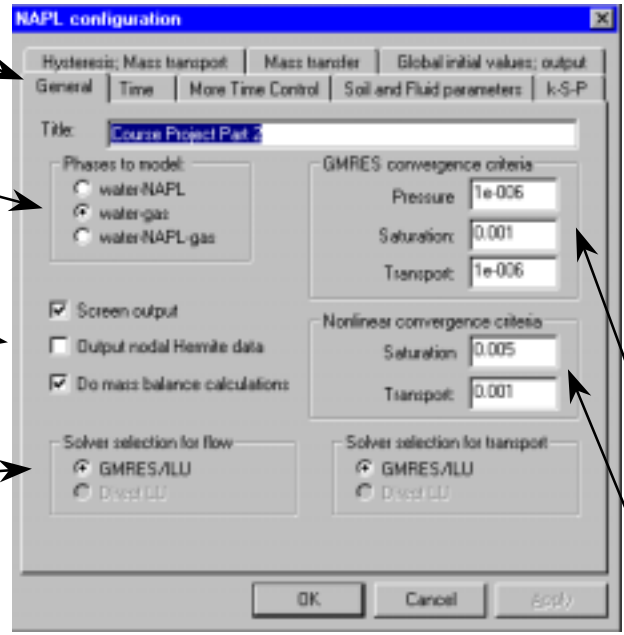
Define model size and solvers (compiler directives):
3 parameters in the file **include.f**
1.) set mesh size
long dimension: *mnnd_l* >= max [nodes in x, nodes in y]
short dimension: *mnnd_s* >= min [nodes in x, nodes in y]
2.) choose solver - (direct = 0, iterative = 1)
itsol_t - solver for transport (concentration, saturation)
itsol_f - solver for flow
3.) number of GMRES solution vector saves
nsave > 1
(as *nsave* increases convergence rate increases **and** memory requirements increase)

General (active)

type of flow problem
2-phase, W-N
2-phase, W-G
3-Phase

output stream
In general keep Hermite data off.

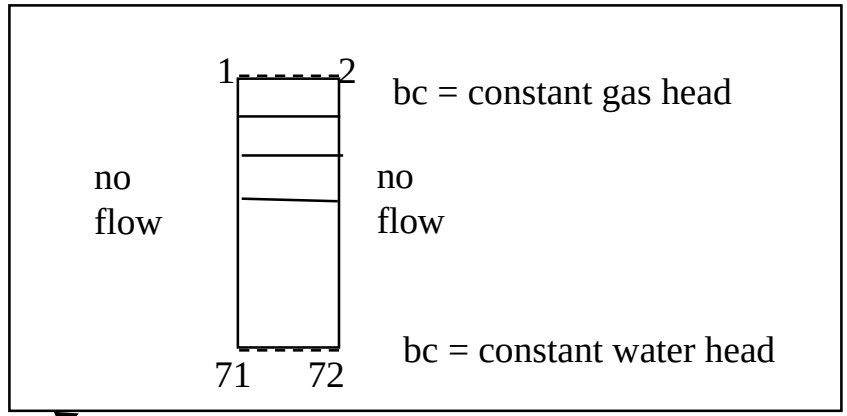
solver selection (not active)
currently a compiler directive (**include.f**)



nonlinear equation convergence criteria (the change in the solution over an iteration step)

GMRES convergence criteria (iterative solver for the linear matrix equation)

Example of screen output:



output during and after a time step for this physical problem

```
- GMRES  (1)

       FLUX CONVERSION for BCs 2, 3, 4 (node, qw, qn, qg)
          1    0.0000E+00    0.0000E+00    4.9891E-03
          2    0.0000E+00    0.0000E+00    4.9891E-03
         71   -4.9891E-03    0.0000E+00    0.0000E+00
         72   -4.9891E-03    0.0000E+00    0.0000E+00

       Tw - GMRES (  1)
       L_S 1     2  0.4995  0.0000  0.5005 (0.035515)  0.090968  0.035515

       Tw - GMRES (  1)
       L_S 2    12  0.9576  0.0000  0.0424 (0.035007)  0.011389  0.005183

       Tw - GMRES (  1)
       L_S 3    13  0.9925  0.0000  0.0075 (0.035135)  0.002949  0.001548


         elapsed time  time step (dt_crit)
           154.616548541857         20.2543324185030         1000.00000000000
           0        39
```

Time

if GMRES takes more than 200 iterations to solve any one matrix equation then the simulator will stop

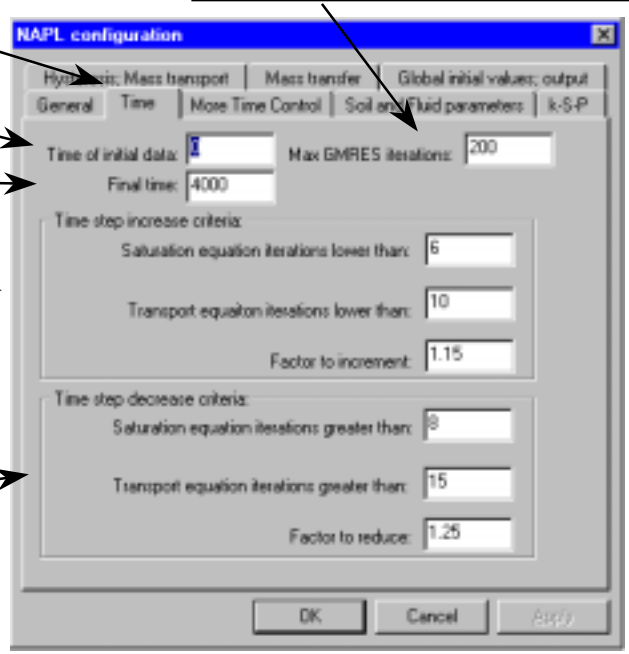
time of initial conditions

time simulation ends

increase the time step by a factor of 1.15 if the number of iterations used to solve the saturation equation is < 6 and transport < 10

decrease the time step by a factor of 1.25 if the number of iterations used to solve the saturation equation is > 8 or transport > 15

otherwise don't change the time step



More Time Control

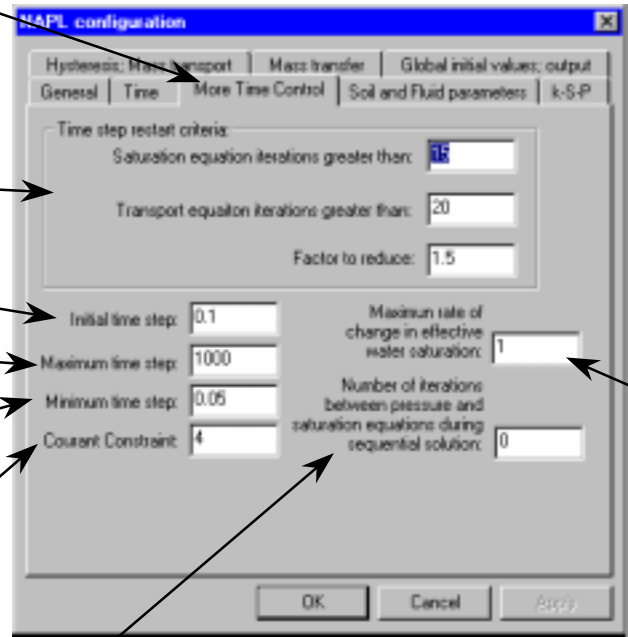
restart the time step and cut it by a factor of 1.5 **if** the number of iterations used to solve the saturation equation is > 15 **or** transport > 20

the time step should start out small to propagate shock-like conditions

either you set the max here, or let the code find the ‘dynamic max’

don’t want them too small or you will either die before finish, or roundoff error will kill you

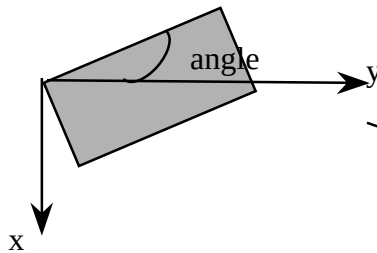
a way to set the max time step based on the ratio of advective transport to grid spacing



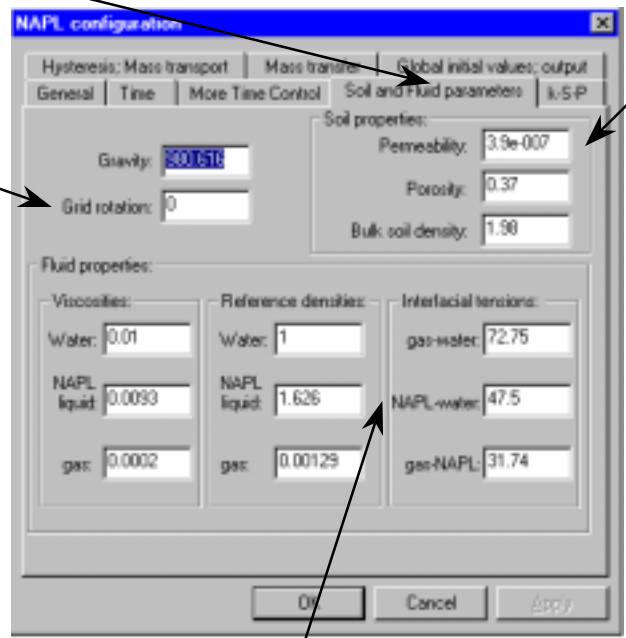
an option for sequential solution of the governing equations (0 = sequential solution, >0 = loop back after each sequential solution

another time step control based on the change in the saturation solution over a time step

Soil and Fluid Parameters



scalar



For capillary pressure scaling

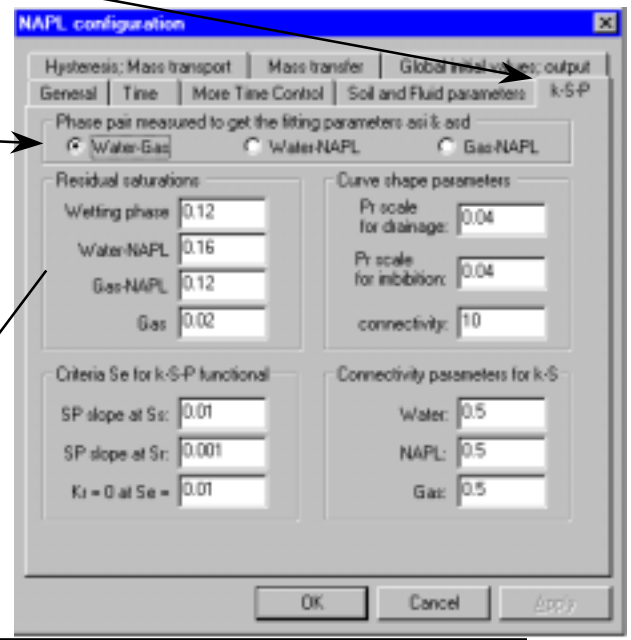
$$\frac{P_{cGW}}{\sigma_{GW}} = \frac{P_{cGN}}{\sigma_{GN}} = \frac{P_{cNW}}{\sigma_{NW}}$$

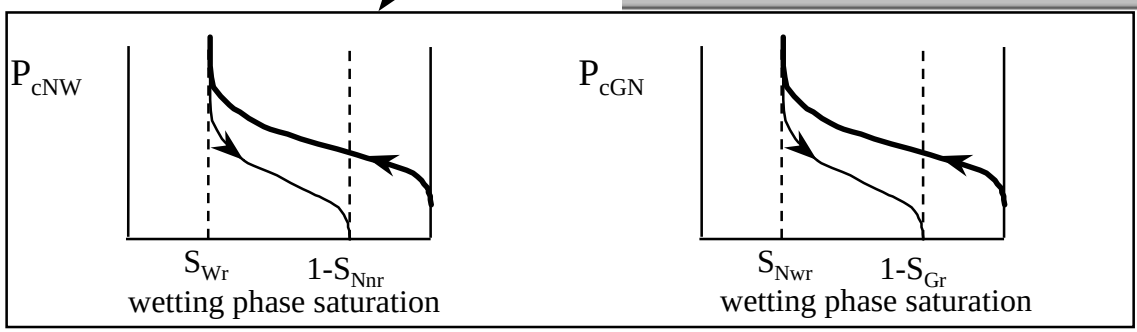
k-S-P

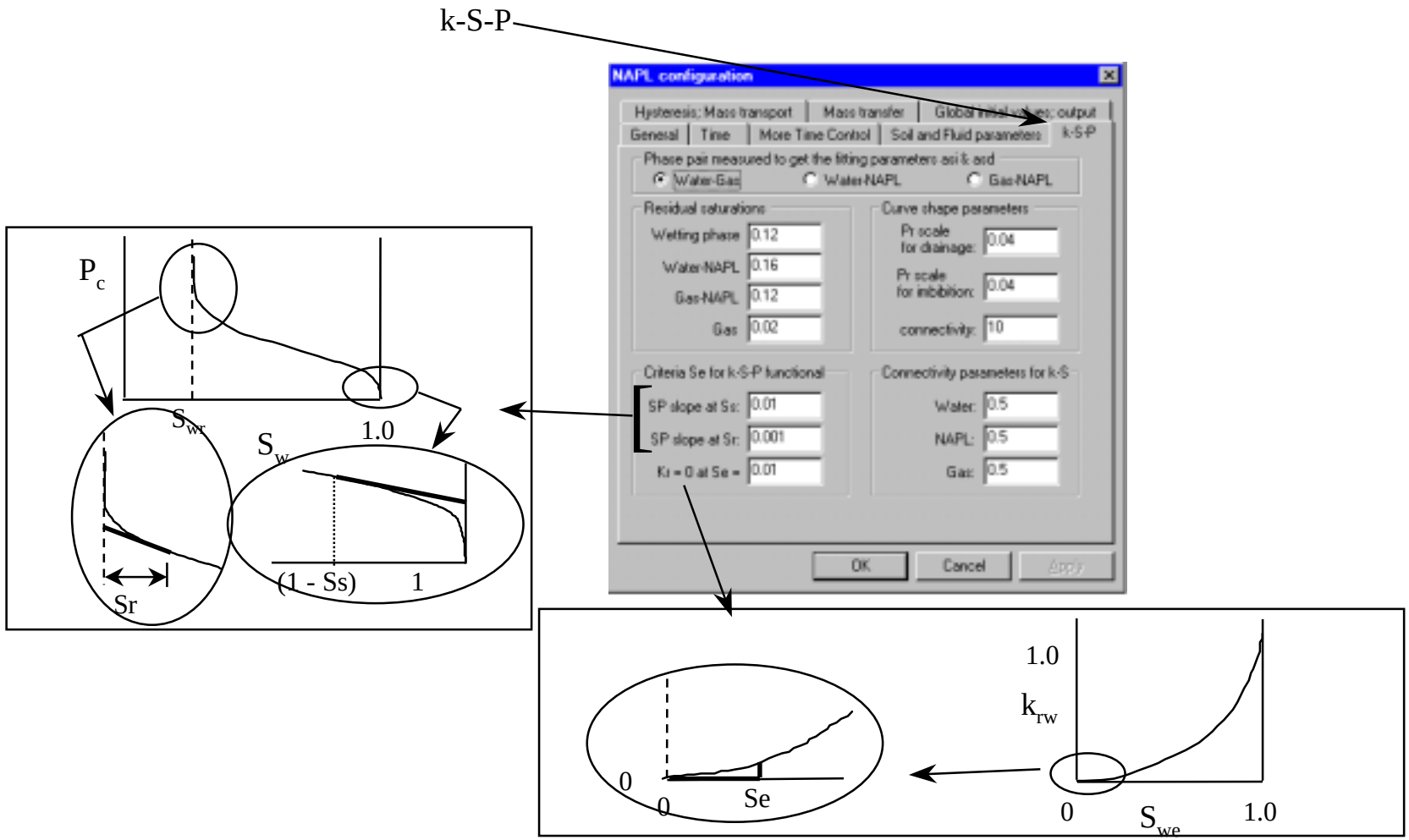
e.g., W-G measured, therefore,

$$P_{cGW}\frac{\sigma_{GN}}{\sigma_{GW}} = P_{cGN}$$

$$P_{cGW}\frac{\sigma_{NW}}{\sigma_{GW}} = P_{cNW}$$



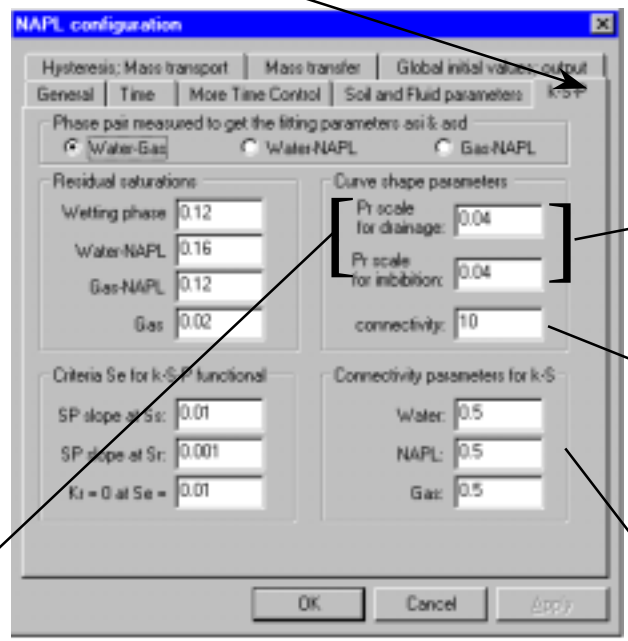


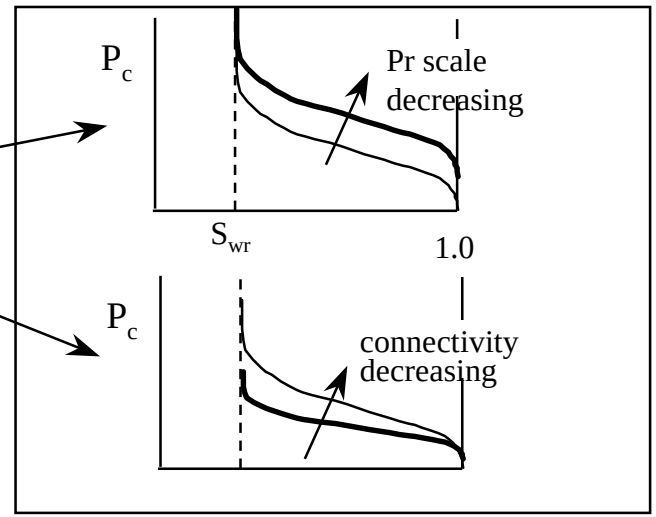


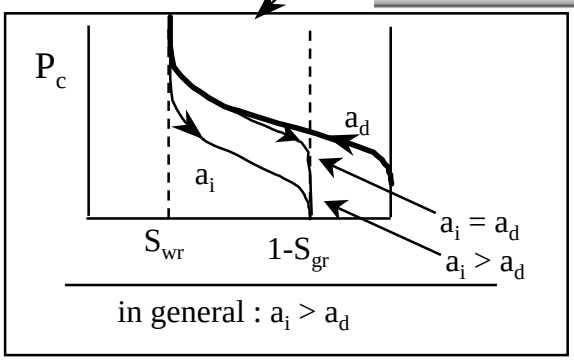
Recall: effective saturation

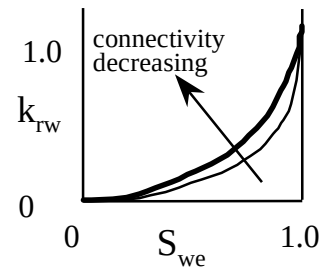
$$S_{ew} = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

k-S-P









$$k_{rw} = S_{ew}^{\varsigma}\left\{1 - \left[1 - S_{ew}^{1/m}\right]^{m}\right\}^{2}$$

$$k_{rg} = S_{eg}^{\varphi}\left\{1 - \left[1 - S_{eg}\right]^{1/m}\right\}^{2m}$$

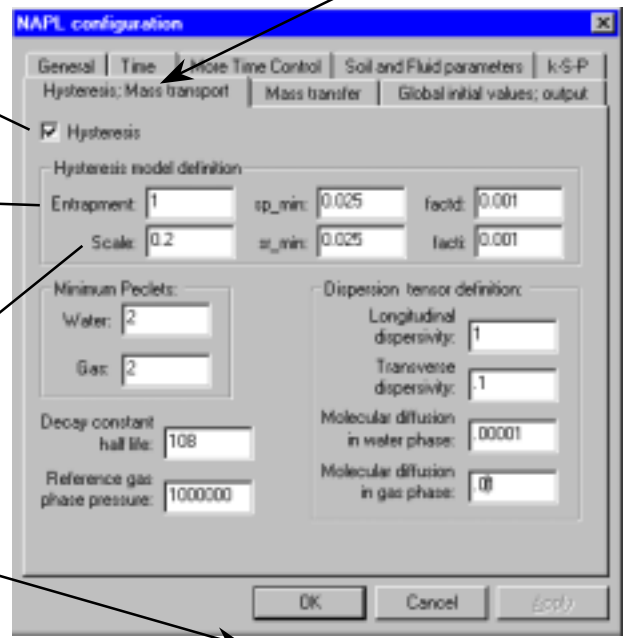
connectivity can be positive or negative, and in general connectivity for the wetting phase is larger than that for the non-wetting phase.

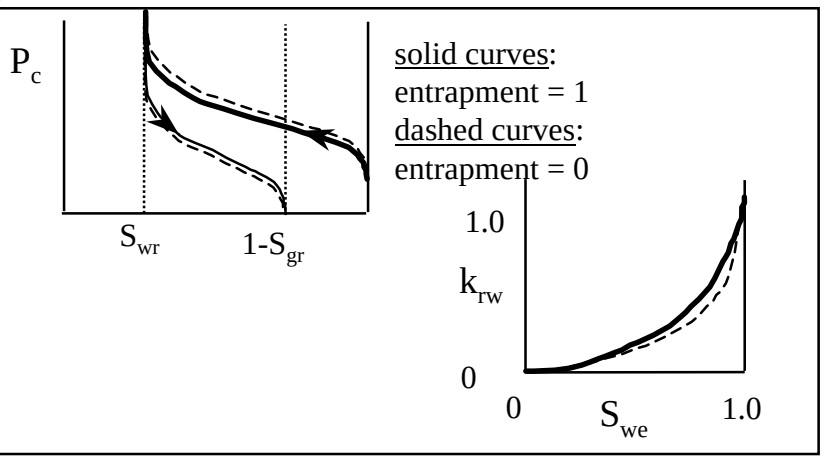
hysteresis on/off option
if on then consider capillary hysteresis and 3-phase fluid entrapment
if off then use only primary drainage curves

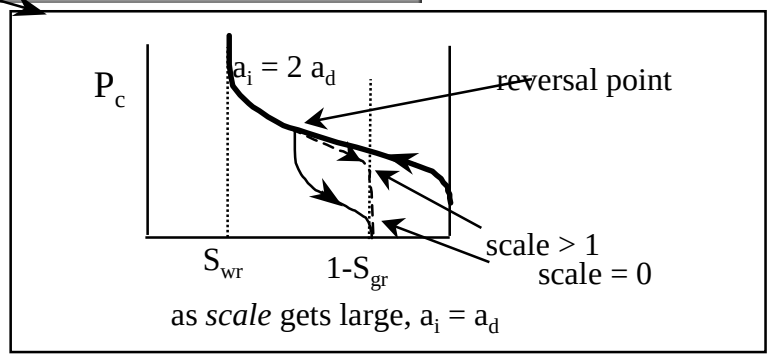
entrapment a blending parameter that defines how fast a phase becomes <u>entrapped during drainage</u> or <u>released during imbibition</u>
1 = linear, 0 = instantaneous

scale: a blending parameter that defines how fast the pressure scale changes after a reversal
(0 = instantaneous)

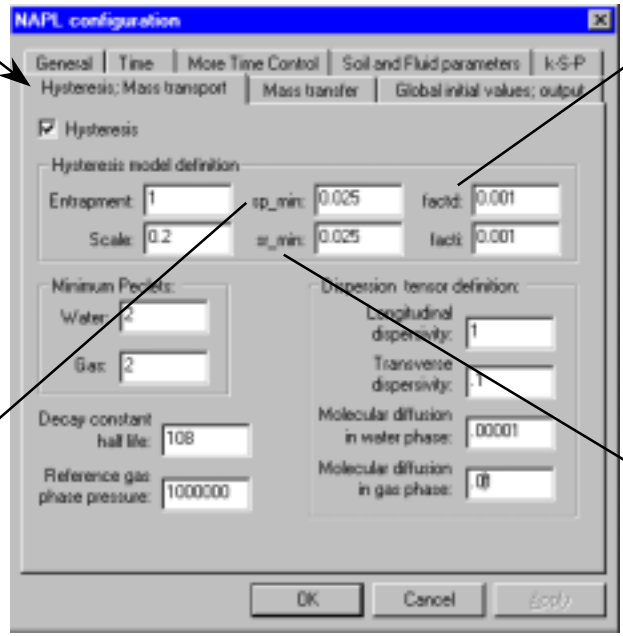
Hysteresis; Mass Transport



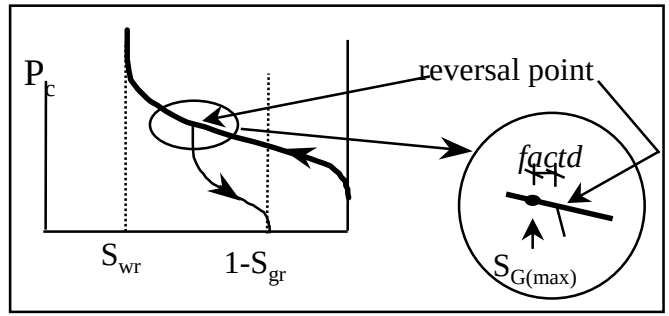




Hysteresis; Mass Transport

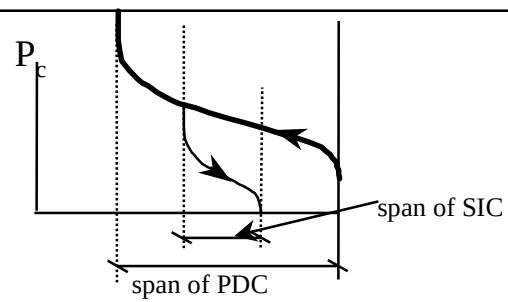


factd, facti
the tolerance in saturation change to initiate reversal



sr_min - saturation must progress at least *sr_min* away from S-P curve endpoint before a reversal will be considered

sp_min - the smallest denominator allowed for effective saturation (the 'span' of the S-P curve
If a reversal will generate a curve that is too 'tight' then keep using the current curve



Recall: effective saturation

$$S_{ew} = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{Gr}} \qquad S_{eG} = \frac{S_G - S_{Gr}}{1 - S_{Wr} - S_{Gr}}$$

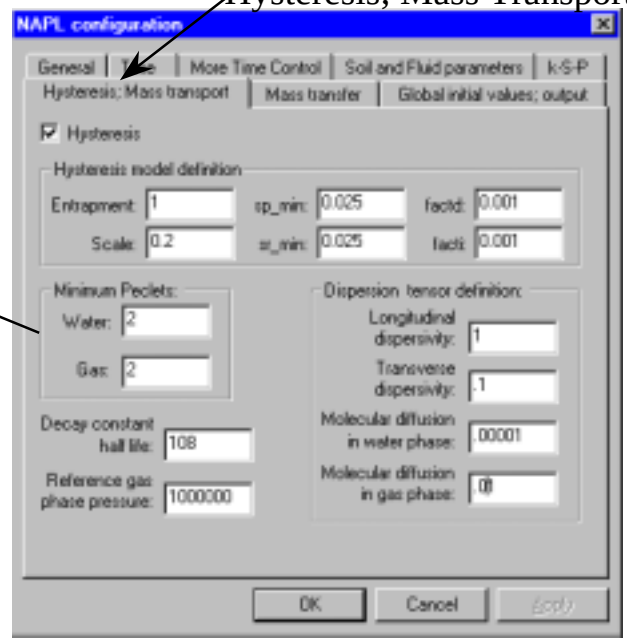
the denominator is the saturation range over which water is mobile

Hysteresis; Mass Transport

Peclet constraint - add artificial diffusion to the phase transport problem when you are using a grid that is too coarse for the S-P parameters chosen.

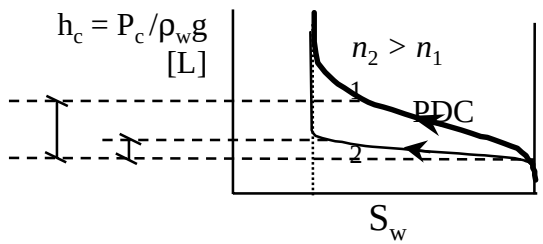
$$Pe = \frac{\text{advection}\ \Delta x}{\text{diffusion}}$$

where diffusion is defined by the slope of the S-P curve. Diffusion is added by forcing the S-P curve to have more slope than is natural. Set this number high to add no artificial diffusion.



Use the PDC to determine the appropriate grid spacing (try to resolve the PDC over 4 elements)

ideal element size
= 1/4 this distance



$$h_c = \frac{\left[S_e^{-1/m} - 1\right]^{1/n}}{a_d}$$

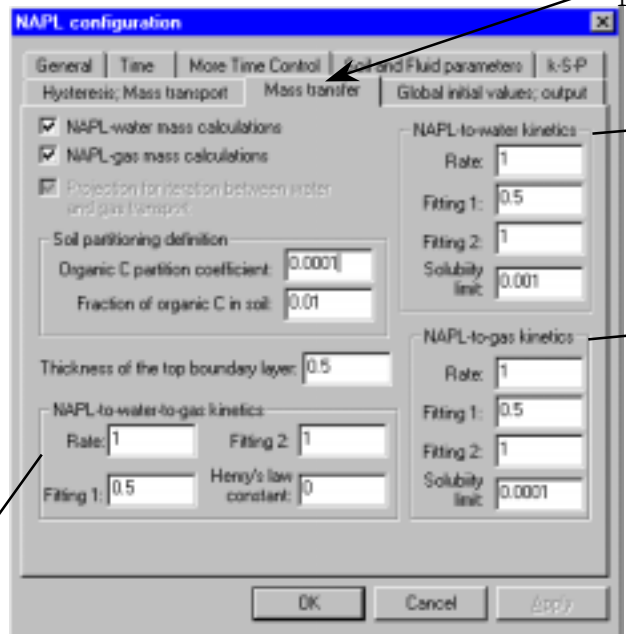
as *n* gets **larger** the *discretization* must get **smaller**

If you can't afford to refine as required, can do 2 things:

1. make *n* smaller than the physical value
2. use a Peclet number around 2.

If you try to resolve the 'front' in too few elements you will get oscillations which may or may not cause problems.

Mass Transfer



Define kinetic mass transfer rule for NAPL dissolving into water

$$K_n^W (C^* - C_n^W)$$

$$K_n^W = R(\theta_N)^{\beta_1} |v_W|^{\beta_2}$$

Define kinetic mass transfer rule for NAPL vaporizing into the gas-phase

$$K_n^G (C^* - C_n^G)$$

$$K_n^G = R(\theta_N)^{\beta_1}$$

Define kinetic mass transfer rule for dissolved NAPL vaporizing into the gas-phase

$$K_{n/W}^G (H C_n^W - C_n^G)$$

$$K_{n/W}^G = R(\theta_W)^{\beta_1}$$

restart option: **yes when checked**.

IC's are read in from the files with an **rs** extension.

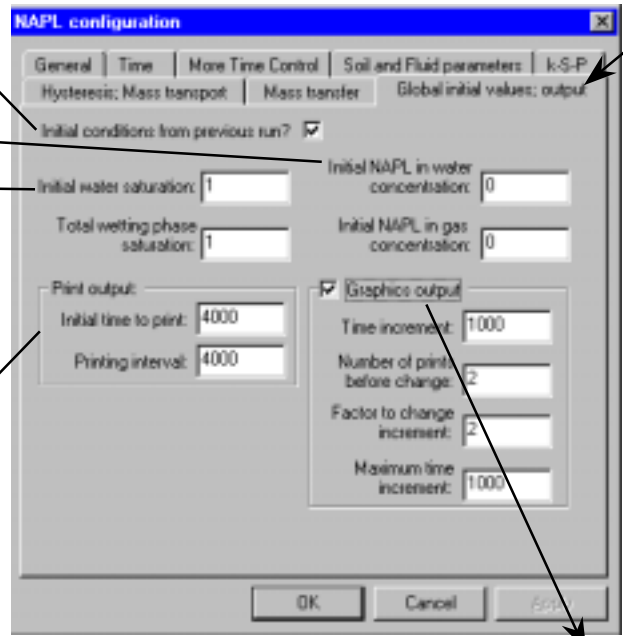
Each time a print interval is executed the **rs** files are 'refreshed' with the solution at that time.

Overrides 'global IC's, but does not override node-specific values.

Global initial values; output

global ICs for saturation and concentration

NEED TO SET THESE VALUES IN THEIR RESPECTIVE LAYERS (4 of them)



Define *print interval*

1. define the time for the first print
2. define the equal time interval to print thereafter

Generates files:

1.) **file1.out, file2.out, …**

has these 7 pieces of data: S_W, S_N, S_G, P_{cNW}, P_{cGN}, ρ_n^W , ρ_n^G

2.) **vel1.out, vel2.out, …**

has these 6 pieces of data: v_{Wx}, v_{Wy}, v_{Nx}, v_{Ny}, v_{Gx}, v_{Gy}

NOT FOR MESHMAKER
keep this off (un-checked)

Point Source/Sink Terms (wells)

Use this condition to input known fluid flux conditions (e.g., water infiltration rate, NAPL application rate, etc.)

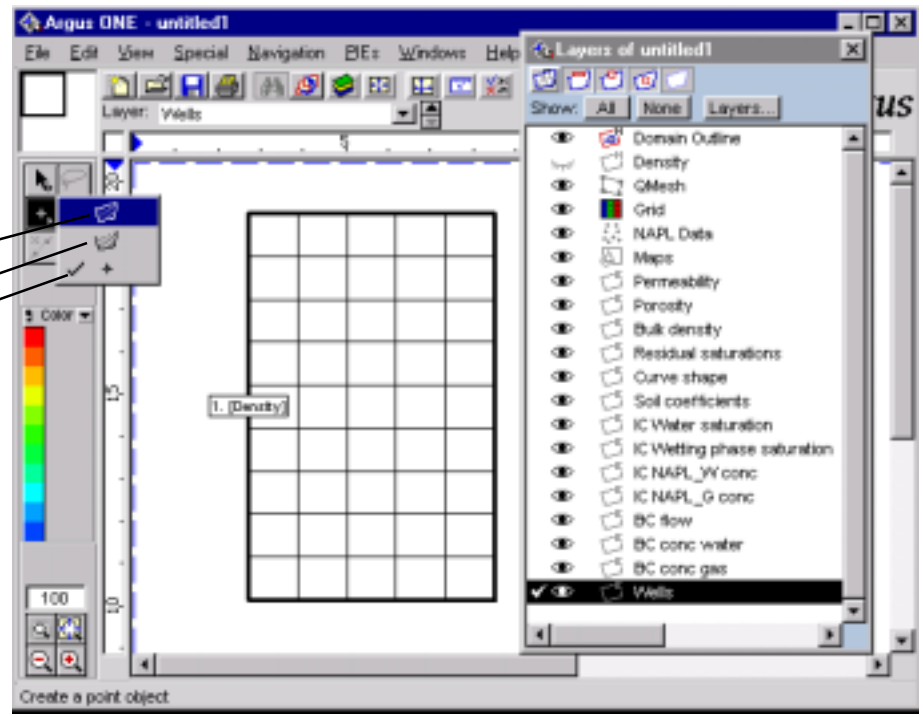
Go to the Wells layer

Choose the tool to apply the well condition at the node.

closed contour

open contour

node



Well condition input window

activate the nodes (= 1)

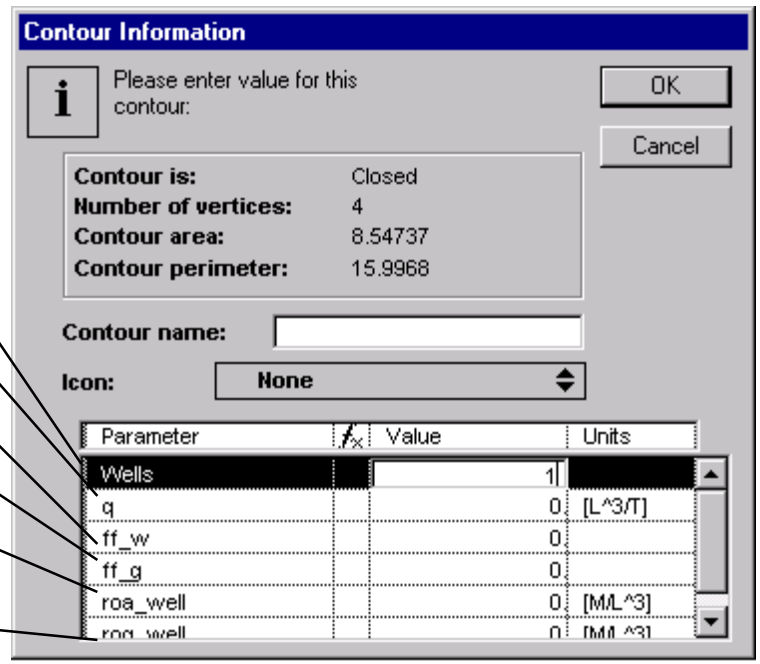
the volumetric flux rate (injection > 0)

the fraction of the total flux that is water

the fraction of the total flux that is gas

the NAPL concentration in the water that is being injected

the the NAPL concentration in the gas that is being injected



Note, at extraction points (q < 0), the distribution of phases and the concentrations are assogned based on the solution.