MODEL I/O

Purpose:

1.) get to know the parameters (what they mean, how to estimate them)

2.) run the model and get a feel for model capability and parameter sensitivity

Approach:

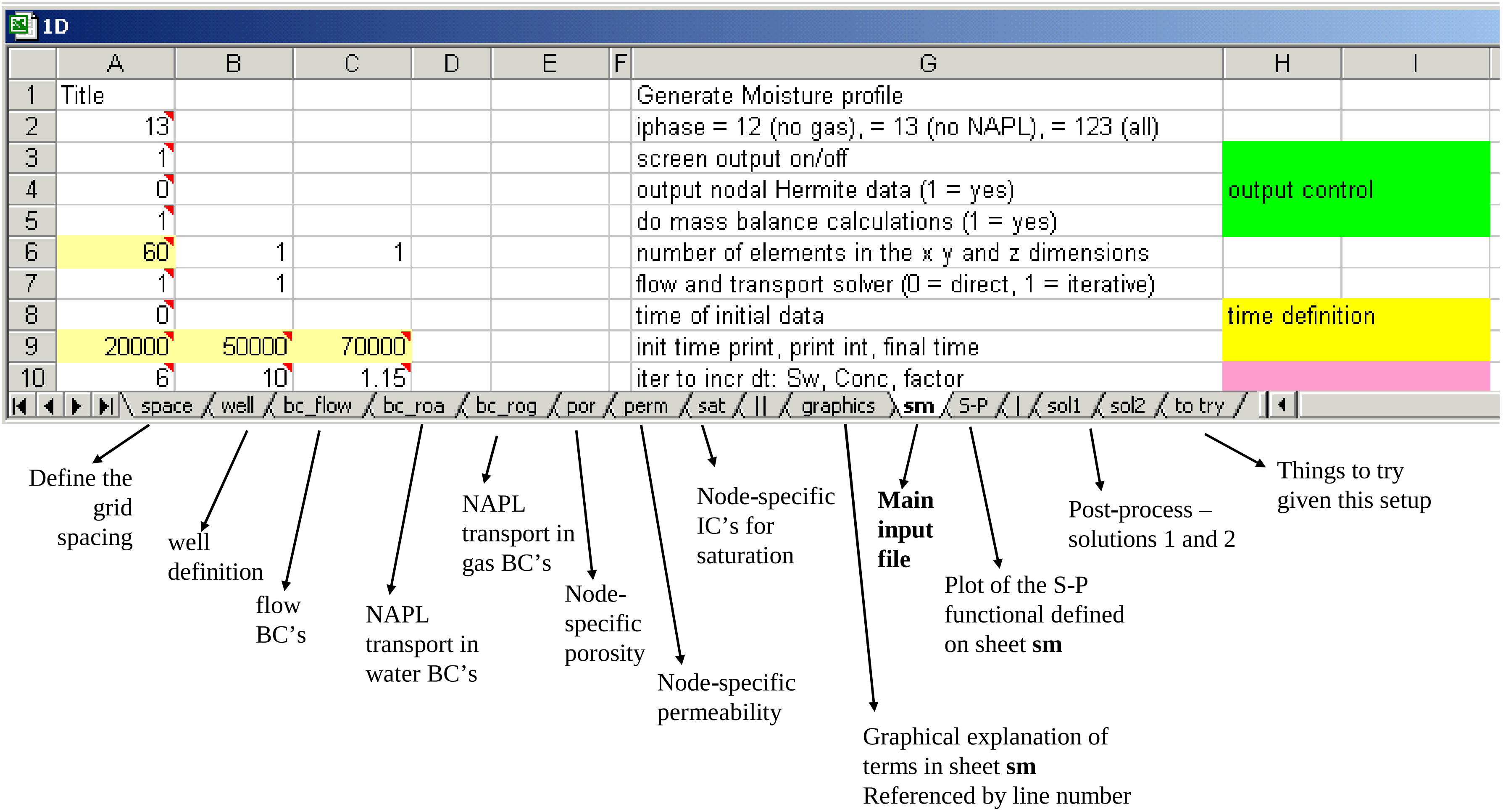
1.) use EXCEL as a pre- and post-processor
Excel (set up a series of 1-D examples) - macros for file export and import

2.) walk through the input files explaining terms

3.) run example problems which highlight features of the model.

EXCEL Pre-processor

Tabs representing the different model input files



Excel file sheet **SM (in parts)**

1	Title					Generate Moisture profile [units cgs]		
2	13					iphase = 12 (no gas), = 13 (no NAPL), = 123 (all)		
3	1					screen output on/off		
4	0					output nodal Hermite data (1 = yes)	output control	
5	1					do mass balance calculations (1 = yes)		
6	60	1	1			number of elements in the x y and z dimensions	grid defiition	
7	0					time of initial data	time definition	
8	50000	50000	100000			init time print, print int, final time		
9	6	10	1.15			iter to incr dt: Sw, Conc, factor		
10	8	15	1.25			iter to decr dt: Sw, Conc, factor	iteration information	
11	15	20	1.5			iter to restart dt: Sw, Conc, factor		
12	200					if iter/dt > itermx, stop		
13	1.25					max ratio of dSew/dt		
14	100					Courant constraint Co = advection *time step / space step		
15	0.1					initial time step	time stepping	
16	1000	0.01				max time step, min time step		
17	0	100	2.00E+00	2	400	grf_on, grinc, ngrch, fgrch, gmax	GMS output control	
18	0					number of iterations between Pw and Sw		
19	0.000001					BiCG Pw convergence criterion		
20	0.001	0.005				BiCG, NL Sw conv criterion	iteration information	
21	0.001	0.001				BiCG, NL Conc. conv criterion		

Excel file sheet **SM**

22	0					=1: list nodes in x and y; =0 list xmax and ymax (sheet **space**)	
23	980.6					gravity magnitude	
24	0	0				grid_rotate,ccw from node 1 about z and y axes, resp	
25	5.00E-07					base permeability	
26	122					number of deviations (in file perm.in)	
27	0.34					base porosity	SOIL PROPERTIES
28	0					number of deviations (in file por.in)	fine grained, well sorted.
29	1.98					bulk soil density	
30	0					number of deviations (in file bulk.in)	
31	0.01	0.005	0.0002			vw_r,vn_r,vg_r	
32	1	1.5	0.0015			rw_r,rn_r,rg_r	FLUID PROPERTIES
33	72.75	39.5	31.74			siggw, signw, siggn	

	A	B	C	D	E	F	G	H
1	1	0.34			* node, porosity			
2	2	0.34						
3	3	0.34						
4	4	0.34						

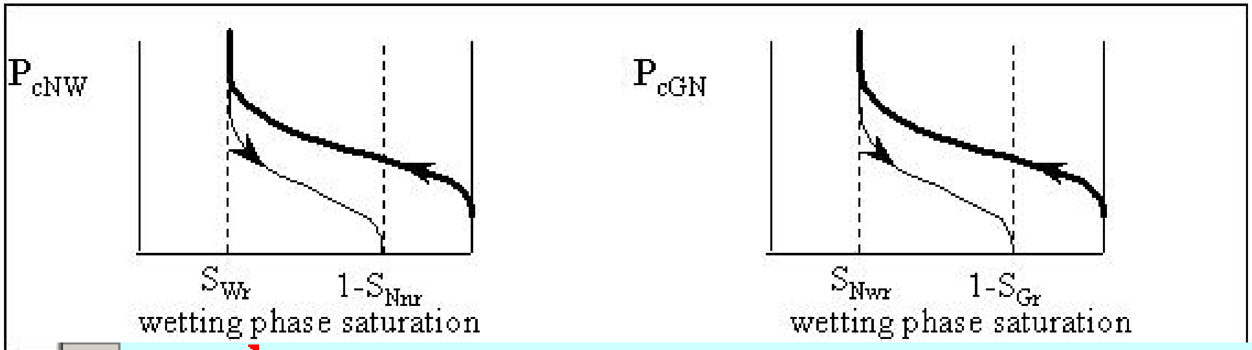
space / well / bc_flow / bc_roa / bc_rog / **por** / perm / sat / || / graphics / sm / S-P / |

	A	B	C	D	E	F	G	H
1	1	5.00E-07		* node, k				
2	2	5.00E-07						
3	3	5.00E-07						
4	4	5.00E-07						

space / well / bc_flow / bc_roa / bc_rog / por / **perm** / sat / || / graphics / sm / S-P / |

	A	B	C	D	E	F	G	H	I
1	1000	2		x max, y max (if input line 23 = 0)				dx =	16.66667
2									
3									
4									

space / well / bc_flow / bc_roa / bc_rog / por / perm / sat / || / graphics / sm / S-P / | / sol1 / sol



when residual saturation = 0 then entrapment hysteresis is ignored

34	1				phase pair measured: =1 G-W, =2 N-W, =3 G-N	
35	0.02	0.15	0.15	0.15	global swr, snnr, snwr, sgr	
36	0				deviations from global	
37	0.007	0.014	2.1		global asd, asi, nsw	
38	0				deviations from global	K-S-P model
39	5E-07	0.34			global soil upon which alpha was based	
40	0				number of deviations in soil-type	
41	0.5	1	1		alfw, nsew1 ,nsew2 shape parameters for k-Sw	
42	0.5	1	3	3	alfn, nsen1 ,nsen2 nsenn3,shape parameters for k-Sw	
43	0.5	1	1		alfg, nseg1 ,nseg2 shape parameters for k-Sw	

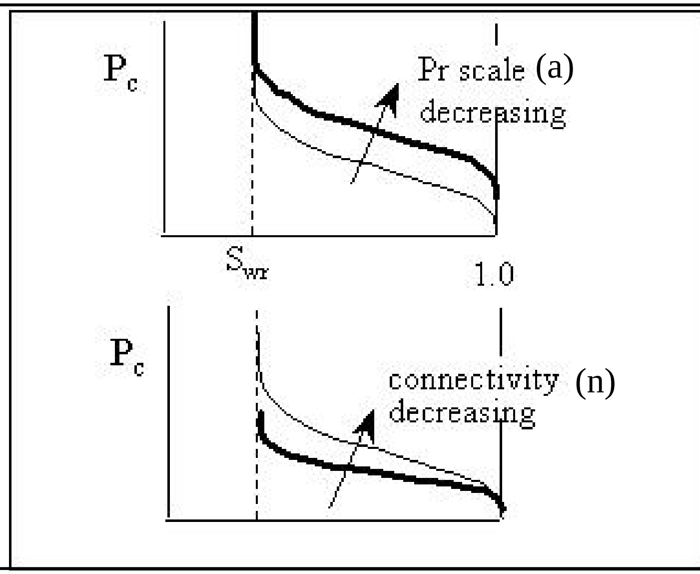
DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /

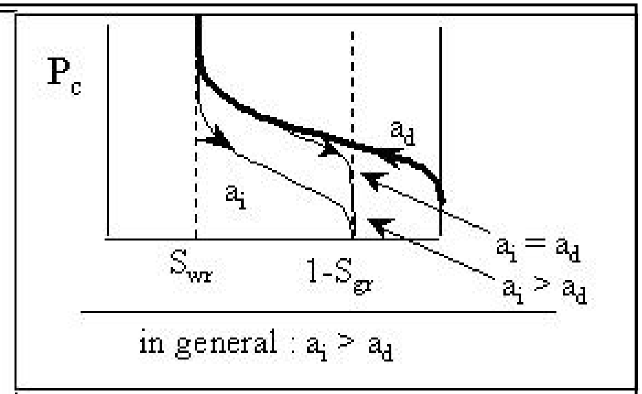
$$h_c\,(S_e) = [\,(S_e)^{-1/m} - 1\,]^{-1/n} \;/\; a$$

$$m = 1 - 1/n$$

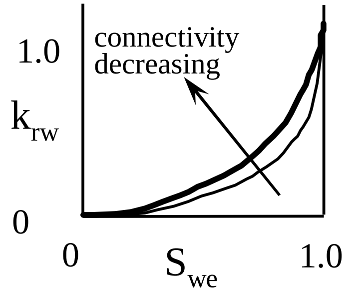
$$h_c = P_c / \rho^W g$$

Effective saturation $S_e = [S - S_r\,] / [S_s - S_r\,]$





when $a_d = a_i$ capillary hysteresis is ignored



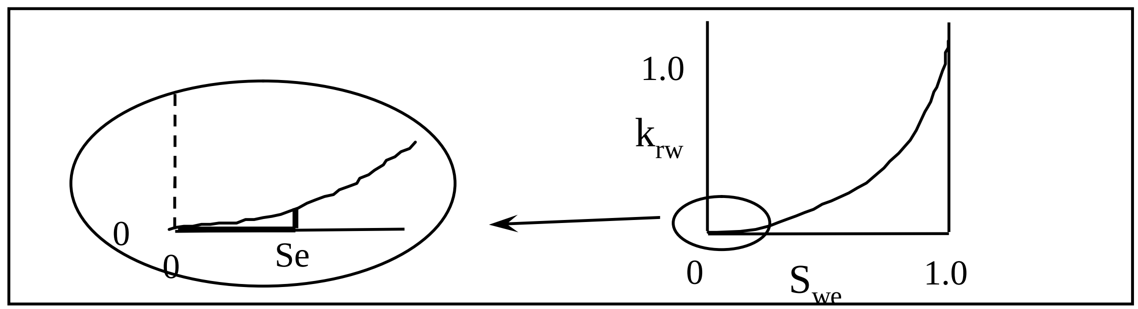
$$k_{rw} = S_{ew}^{\varsigma}\left\{1 - \left[1 - S_{ew}^{1/m}\right]^{m}\right\}^{2}$$

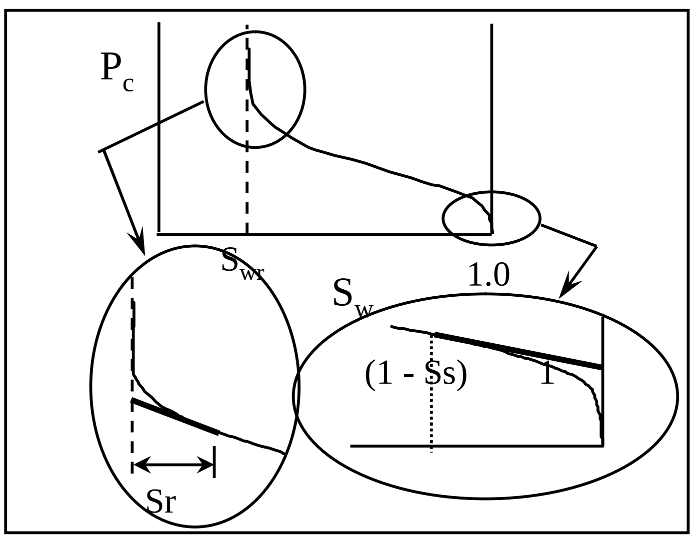
$$k_{rg} = S_{eg}^{\varphi}\left\{1 - \left[1 - S_{eg}\right]^{1/m}\right\}^{2m}$$

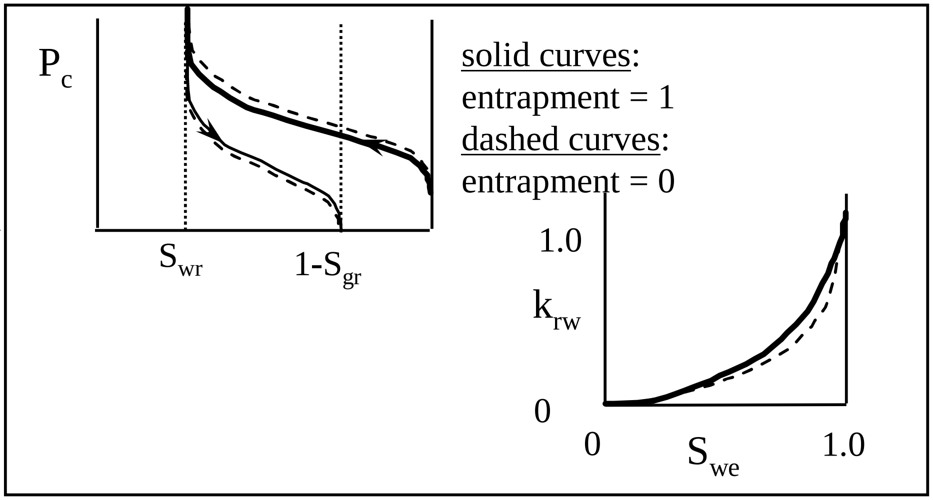
connectivity can be positive or negative, and in general connectivity for the wetting phase is larger than that for the non-wetting phase.

34	1				phase pair measured: =1 G-W, =2 N-W, =3 G-N	
35	0.02	0.15	0.15	0.15	global swr, snnr, snwr, sgr	
36	0				deviations from global	
37	0.007	0.014	2.1		global asd, asi, nsw	
38	0				deviations from global	K-S-P model
39	5E-07	0.34			global soil upon which alpha was based	
40	0				number of deviations in soil-type	
41	0.5	1	1		alfw, nsew1 ,nsew2 shape parameters for k-Sw	
42	0.5	1	3	3	alfn, nsen1 ,nsen2 nsenn3,shape parameters for k-Sw	
43	0.5	1	1		alfg, nseg1 ,nseg2 shape parameters for k-Sw	
44	0.01	0.001			se_s, se_r, limit values of dPc/dS	
45	0.01				sfact_kr, limit values of Kr	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /

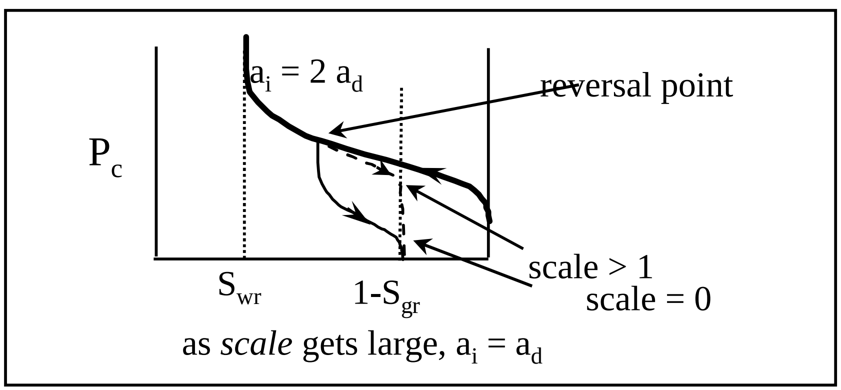




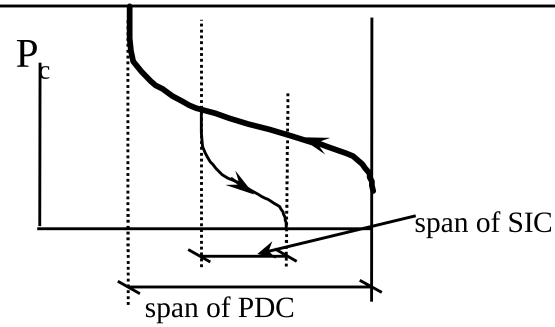


38	0				deviations from global	K-S-P model
39	5E-07	0.34			global soil upon which alpha was based	
40	0				number of deviations in soil-type	
41	0.5	1	1		alfw, nsew1 ,nsew2 shape parameters for k-Sw	
42	0.5	1	3	3	alfn, nsen1 ,nsen2 nsenn3,shape parameters for k-Sw	
43	0.5	1	1		alfg, nseg1 ,nseg2 shape parameters for k-Sw	
44	0.01	0.001			se_s, se_r, limit values of dPc/dS	
45	0.01				sfact_kr, limit values of Kr	
46	1				hysteresis on? 1=yes	
47	1				entrapment e_r, d/i (>= 0) 0=instantaneous	
48	0.2				b_a, power for alpha chg (>=0)	
49	0.05	0.075			sp_min, sr_min, curve restriction parameters	
50	0.001	0.001			factd,facti, reversal tolerance, dr,im	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /



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

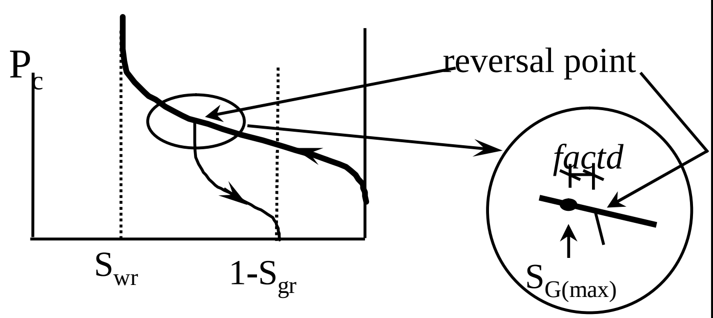


sr_min - saturation must progress at least *sr_min* away from S-P curve endpoint before a reversal will be considered

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

38	0				deviations from global	K-S-P model
39	5E-07	0.34			global soil upon which alpha was based	
40	0				number of deviations in soil-type	
41	0.5	1	1		alfw, nsew1,nsew2 shape parameters for k-Sw	
42	0.5	1	3	3	alfn, nsen1,nsen2 nsenn3,shape parameters for k-Sw	
43	0.5	1	1		alfg, nseg1,nseg2 shape parameters for k-Sw	
44	0.01	0.001			se_s, se_r, limit values of dPc/dS	
45	0.01				sfact_kr, limit values of Kr	
46	1				hysteresis on? 1=yes	
47	1				entrapment e_r, d/i (>= 0) 0=instantaneous	
48	0.2				b_a, power for alpha chg (>=0)	
49	0.05	0.075			sp_min, sr_min, curve restriction parameters	
50	0.001	0.001			factd,facti, reversal tolerance, dr,im	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /



49	0.05	0.075				sp_min, sr_min, curve restriction parameters		
50	0.001	0.001				factd,facti, reversal tolerance, dr,im		
51	200	200				minimum peclet number: water, gas		

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /

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.

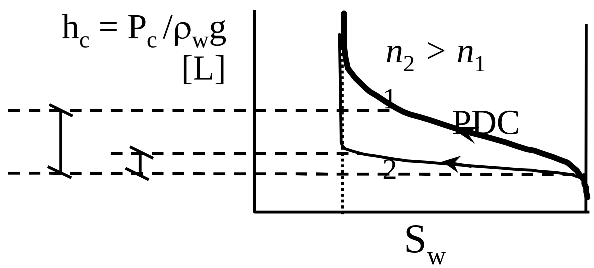
$$Pe = \frac{advection \, \Delta x}{diffusion}$$

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.

set high (~200) to turn off, set to ~2 to turn on full

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

ideal element size
= 1/4 this distance



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

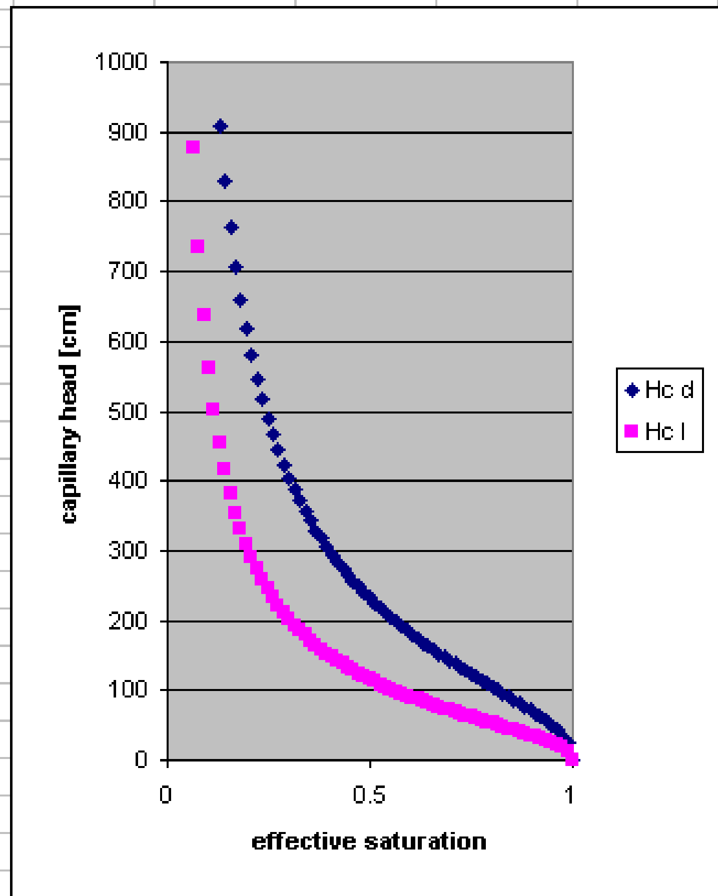
If you can’t afford to refine as required, can do 2 things:
1. make *n* smaller than the physical value
2. use a Peclet number around 2.

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

Sheet S-P is a plot of the PDC for the parameters defined in line 37 (ai, ad and n)

Linked to sheet **sm**, plot automatically refreshed.

1	Compute the S-P curve for 2 paris of fitting parameters				(n, a)			
2		Se	Hc d	Hc l	m	n	ad	ad
3	1	1	0	0	0.52381	2.1	0.007	0.014
4	0.99	0.986807	24.9774	12.4887				
5	0.98	0.973615	35.07162	17.53581				
6	0.97	0.960422	42.94707	21.47353				
7	0.96	0.94723	49.73002	24.86501				
8	0.95	0.934037	55.85015	27.92508				
9	0.94	0.920844	61.52584	30.76292				
10	0.93	0.907652	66.88623	33.44311				
11	0.92	0.894459	72.01546	36.00773				
12	0.91	0.881266	76.97228	38.48614				
13	0.9	0.868074	81.79989	40.89995				
14	0.89	0.854881	86.53148	43.26574				
15	0.88	0.841689	91.1934	45.5967				
16	0.87	0.828496	95.80728	47.90364				
17	0.86	0.815303	100.3913	50.19566				
18	0.85	0.802111	104.9612	52.48062				
19	0.84	0.788918	109.531	54.76548				
20	0.83	0.775726	114.113	57.0565				
21	0.82	0.762533	118.7189	59.35945				
22	0.81	0.74934	123.3595	61.67973				
23	0.8	0.736148	128.045	64.02249				
24	0.79	0.722955	132.7854	66.39271				
25	0.78	0.709763	137.5906	68.79528				
26	0.77	0.69657	142.4701	71.23505				
27	0.76	0.683377	147.4339	73.71693				
28	0.75	0.670185	152.4917	76.24586				



space / well / bc_flow / bc_roa / bc_rog / por / perm / sat / || / graphics / sm / S-P / | / sol1 / sol2 / to try /

53	0	0			ntr_ow, ntr_og , 1=yes	
54	1				projection for NAPL-in-water to gas	
55	1.00E+00	0.2	0.00001	0.009	along atran diffw diffg	
56	123	0			soil partitioning definition (Koc and Foc)	
57	0				deviations for organic carbon	
58	0.5				thickness of the top boundary layer	Transport parameters
59	10	0.5	1		rate coeff. def. for NAPL to water	
60	0.05				sol. limit (g/cm^3) for NAPL to water	
61	1.16E-05	1			rate coeff. def. for NAPL to gas	
62	0				sol. limit (g/cm^3) for NAPL to gas	
63	0.000116	1			rate coeff. def. for diss. NAPL to gas	
64	0.236				Henry's law constant	
65	0				decay constant half life [day]	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try

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

$$K^G_{n/W}\,(H\,C^W_n - C^G_n)$$

$$K^G_{n/W} = R\,(\theta_W)^{\beta_1}$$

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

$$K^G_n\,(C^* - C^G_n)$$

$$K^G_n = R\,(\theta_N)^{\beta_1}$$

Define kinetic mass transfer rule for NAPL dissolving into water

$$K^W_n\,(C^* - C^W_n)$$

$$K^W_n = R\,(\theta_N)^{\beta_1}\,|v_W|^{\beta_2}$$

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.

66	1	global initial Sw	
67	1	global initial St	
68	0	global initial NAPL in water conc.	
69	0	global initial NAPL in gas conc.	Initial conditions
70	0	initial conditions from a previous run? 1=yes	
71	0	# of nobal changes from global Sw & St IC	
72	0	# of nobal changes from global N/W Conc IC	
73	0	# of nobal changes from global N/G Conc IC	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / **sm** / S-P / | / temp / sol1 / sol2 / to try /

If entry >0 then, list nodal values here.

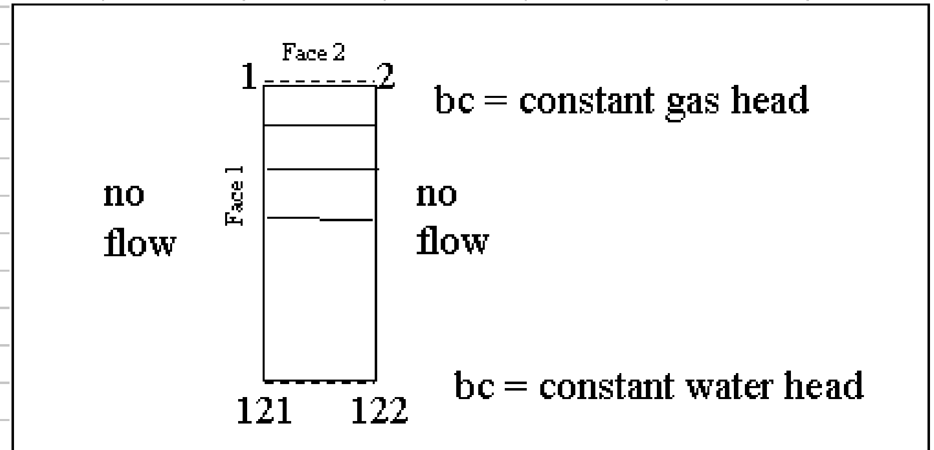
1	1	1	1	* node, Sw, St
2	2	1	1	
3	3	1	1	
4	4	1	1	
5	5	1	1	
6	6	1	1	
7	7	1	1	
8	8	1	1	
9	9	1	1	
10	10	1	1	
11	11	1	1	
12	12	1	1	
13	13	1	1	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / **sw** / || / graphics / sm / S-P / | / temp / sol1 / sol2 / to try /

stress 1

stress 2

	A	B	C	D	E	F	G	H	I	J	K
1	2	1	2			* stress 1		nface, node, bc code			
2	0							head			
3	2	2	2								
4	0										
5	2	121	4								
6	300										
7	2	122	4								
8	300										
9	2	1	2								
10	0										
11	2	2	2								
12	0										
13	2	121	4								
14	300										
15	2	122	4								
16	300										



space / well / bc_flow / bc_roa / bc_rog / por / perm / sat / || / graphics / sm / S-P / | / sol1 / sol2 / to try /

74	0					number of Roa Dirichlet BC's	
75	0					number of Rog Dirichlet BC's	BCs for the first stress period
76	4					number of Dirichlet BC's for FLOW	
77	0					number of point source nodes	
78	100000	13	1	1000	1000	timec, iphase, initial dt, max dt, co	end of period and setup for next
79	0					number of Roa Dirichlet BC's	
80	0					number of Rog Dirichlet BC's	BCs for the second stress period
81	4					number of Dirichlet BC's for FLOW	
82	2					number of point source nodes	
83	10000000	13	1	1000	1000	timec, iphase, initial dt, max dt, co	

DOC / space / well / bc_flow / bc_roa / bc_rog / por / perm / sw / || / graphics / sm / S-P / | / temp / sol1 / sol2 / to try /

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	3	0.0006	1	0	0	0	node,	rate,	ff_w,	ff_g,	c_d,	c_v		20.40945	in/d
2	4	0.0006	1	0	0	0	node,	rate,	ff_w,	ff_g,	c_d,	c_v			

space / well / bc_flow / bc_roa / bc_rog / por / perm / sat / || / graphics / sm / S-P / | / sol1 / sol2 / to try /

OUTPUT FILES

Category:

<u>Restart files</u>: extension **.rs**

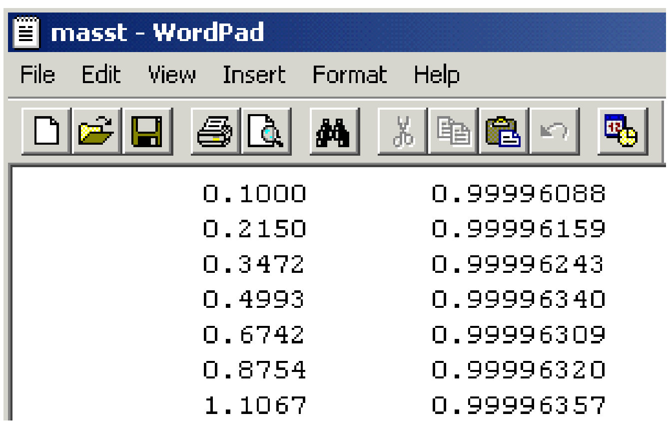
refreshed every time the solution is printed.

<u>Mass balance files</u>:

cmass.out – cumulative mass balance for each phase after each time step

mass.out – mass balance summary for each solution print interval.

masst.out – total mass balance



0.1000	0.99996088
0.2150	0.99996159
0.3472	0.99996243
0.4993	0.99996340
0.6742	0.99996309
0.8754	0.99996320
1.1067	0.99996357

Time

mass balance ratio over time step (1 = perfect)

OUTPUT FILES

Category:

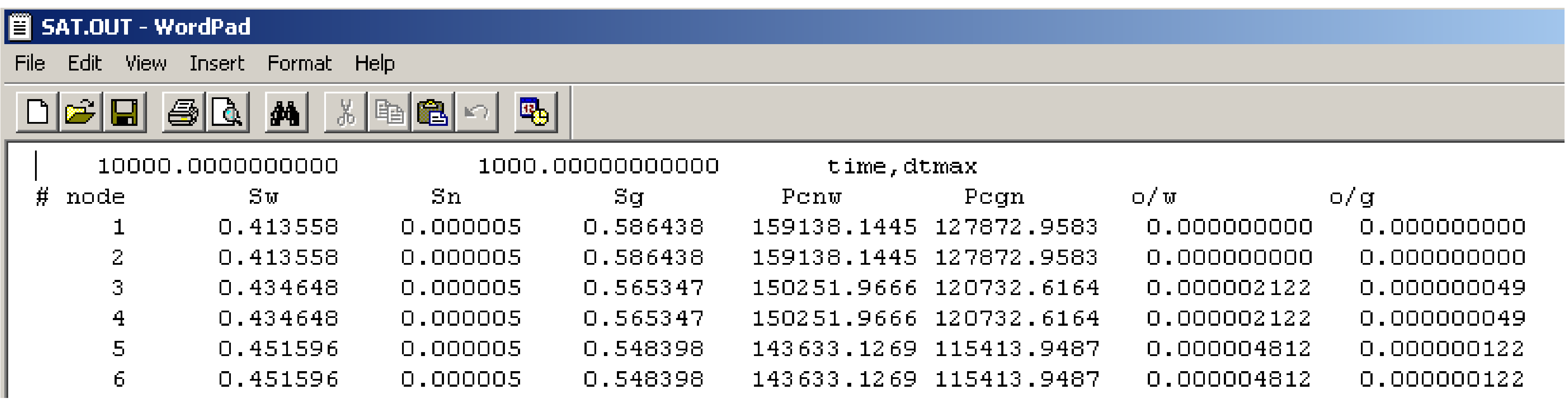
<u>Solution files:</u>

Hermite data (if enabled): at each node, the function and its spatial derivatives
sw.out, st.out, pa.out, oa.out, og.out

Solution at the nodes: **sat.out** (Sw, Sn, Sg, Pcnw, Pcgn, roa, rog)
velw.out, veln.out, velg.out (phase velocity components)

Solution files related to Excel:
for each print interval a separate file is generated and numbered appropriately:

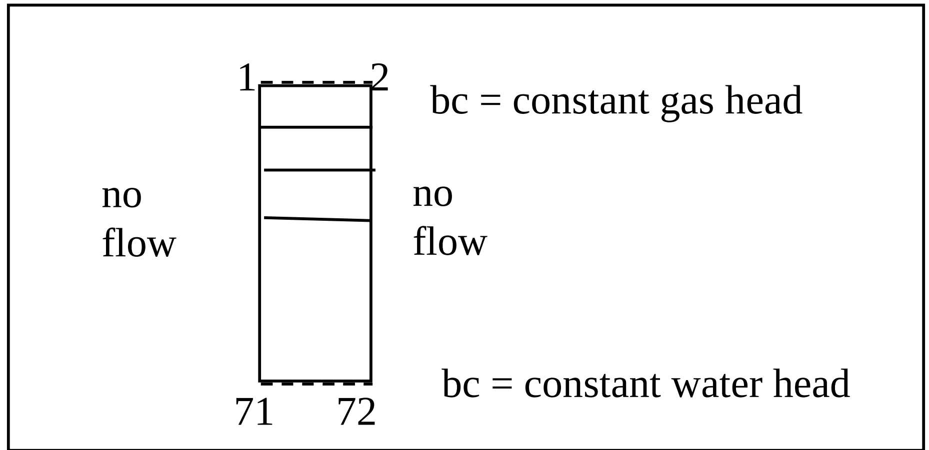
sat.out : Sw, Sn, Sg, Pcnw, Pcgn, roa, rog



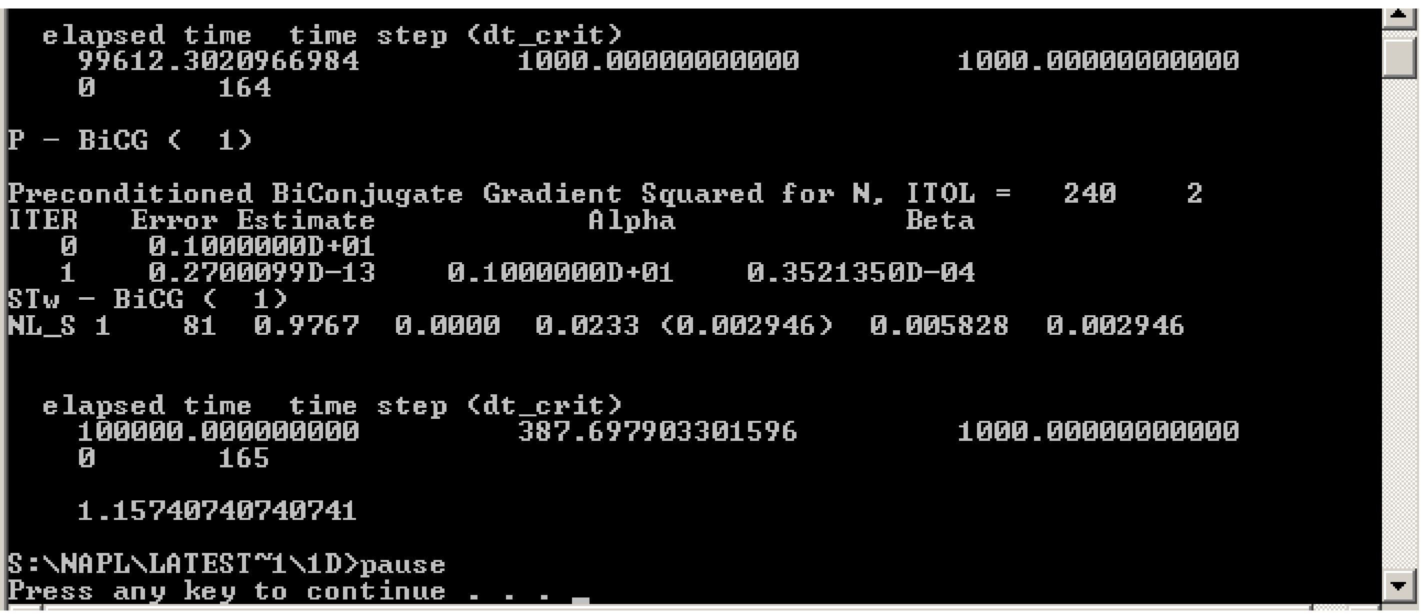
10000.0000000000 1000.00000000000 time,dtmax

# node	Sw	Sn	Sg	Pcnw	Pcgn	o/w	o/g
1	0.413558	0.000005	0.586438	159138.1445	127872.9583	0.000000000	0.000000000
2	0.413558	0.000005	0.586438	159138.1445	127872.9583	0.000000000	0.000000000
3	0.434648	0.000005	0.565347	150251.9666	120732.6164	0.000002122	0.000000049
4	0.434648	0.000005	0.565347	150251.9666	120732.6164	0.000002122	0.000000049
5	0.451596	0.000005	0.548398	143633.1269	115413.9487	0.000004812	0.000000122
6	0.451596	0.000005	0.548398	143633.1269	115413.9487	0.000004812	0.000000122

Example of screen output:



output during and after a time step for this physical problem



```
  elapsed time  time step (dt_crit)
    99612.3020966984         1000.00000000000         1000.00000000000
    0       164

P - BiCG (  1)

Preconditioned BiConjugate Gradient Squared for N, ITOL =   240    2
ITER   Error Estimate             Alpha               Beta
   0    0.1000000D+01
   1    0.2700099D-13    0.1000000D+01    0.3521350D-04
STw - BiCG (  1)
NL_S 1    81  0.9767  0.0000  0.0233 (0.002946)  0.005828  0.002946


  elapsed time  time step (dt_crit)
    100000.000000000         387.697903301596         1000.00000000000
    0       165

    1.15740740740741

S:\NAPL\LATEST~1\1D>pause
Press any key to continue . . .
```

Saturation convergence info:
- it #,
- node of largest change,
- Sw, Sn, Sg at that node,
- (max ΔS over time step)
- L2 norm of nonlinear convergence
- L∞ norm of nonlinear convergence

Time information
- elapsed time (units specified in input)
- Δt for last time step
- max Δt allowed (specified in input file)
- # time step restarts due to lack of convergence
- # time steps since beginning

EXAMPLE PROBLEMS
Using the EXCEL interface

1.) moisture profile
2.) DNAPL flood
3.) dissolution of residual DNAPL
4.) dissolution and vaporization of residual DNAPL

See file 1D.ppt