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Users Guide for SIMSOL (Version 1.0)

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Users Guide for SIMSOL
(Version 1.0)

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I. INTRODUCTION

SIMSOL calculates temperature, pressure, saturation, and air-mass fraction in a uniform geologic medium surrounding a linear heat source. The theory on which this program is based is described in the papers "A similarity solution for two-phase fluid and heat flow near high-level nuclear waste packages emplaced in porous media" [*Doughty and Pruess*, 1990] and "A similarity solution for two-phase water, air, and heat flow near a linear heat source in a porous medium" [*Doughty and Pruess*, 1991]. This users guide does not duplicate the information contained in these two papers, and will be difficult to read without a knowledge of their content.

A flow chart for SIMSOL is shown in Figure 1. The input for SIMSOL is described in Section II, followed by guidelines for running the program in Section III, and listings of input and output files for sample calculations in Section IV. Numerous examples of the graphical output of SIMSOL may be found in *Doughty and Pruess* [1990, 1991].

SIMSOL is written in FORTRAN. It was developed on a Cray 2 at the National Energy Research Supercomputer Center (NERSC) at Lawrence Livermore National Laboratory (LLNL). It has also been tested on a Cray X-MP at NERSC and a VAX 6420 running VMS at Lawrence Berkeley Laboratory (LBL). The equation of state subroutines that describe thermophysical fluid properties as a function of temperature and pressure are essentially the same as those found in the numerical simulator TOUGH2 [*Pruess*, 1987, 1991]. The SIMSOL algorithm allows the specification of a linear heat sink or mass source or sink as well as a linear heat source, but these options have not been tested.

The SIMSOL source code and sample-calculation files are available on diskette or tape.

II. INPUT DESCRIPTION

1. Choice of Shooting Variables and Integration Options

IFX1 IFX2 NZ IBAT IVPL ILOG IDEL

FORMAT (7I5)

IFX1 flag identifying single-phase variable to shoot with (in addition to P and T):

- 0 air partial pressure (P_a)
- 1 air mass fraction (in gas or liquid phase) (X_g^a or X_l^a)
- 2 log of air partial pressure ($\ln(P_a)$)

IFX2 flag identifying two-phase variable to shoot with (in addition to P and S_g):

- 0 air partial pressure (P_a)
- 1 air mass fraction in gas phase (X_g^a)
- 2 log of air partial pressure ($\ln(P_a)$)
- 3 temperature (T)

NZ maximum number of points to save in file PLOT during integration from ZL to ZU; program only saves points a distance (ZU - ZL)/NZ apart; maximum value of NZ allowed is 400; use NZ = 0 to save the first 399 steps and the last step.

IBAT interactive/batch mode flag

- 0 use interactive mode: program prompts for further action after each section; if integration goes out of range in EOS (equation of state) in Preshoot Section, user is prompted for corrective action
- 1 use batch mode: no prompting, if integration goes out of range in EOS, program stops; generally used when initial guess is close to correct answer and Newton-Raphson is unlikely to get into trouble

IVPL vapor pressure lowering flag

- 0 no vapor pressure lowering
- 1 vapor pressure lowering
- -1 vapor pressure lowering, with 'unlowered' vapor pressure used for determining liquid density and internal energy, since these functions may not be defined for T, P conditions accompanying strong vapor pressure lowering
  Warning: IVPL = -1 does not presently work
- 2 no vapor pressure lowering, but use matrix solution scheme in DERIVS (should give identical results to IVPL = 0)

ILOG flag identifying the output form of P_a

- 0 write air partial pressure, P_a, in file PLOT
- 1 write log air partial pressure, $\ln(P_a)$, in file PLOT (ILOG=0 is used for problems without air, regardless of what is input)

IDEL flag determining phases changes that may occur as integration proceeds from ZL to ZU ($r=0$ to $r=\infty$, or $t=\infty$ to $t=0$):

- 1 gas $\rightarrow$ two-phase and two-phase $\rightarrow$ liquid (example: heat source at ZL)
- -1 liquid $\rightarrow$ two-phase and two-phase $\rightarrow$ gas (example: heat sink at ZL)
  Warning: IDEL = -1 has not been tested

Notes on the choice of IFX1 and IFX2:

1) For all values of IFX1 and IFX2, P_a is used as the primary variable during the integration; the IFX flag identifies the variables used to specify boundary conditions (i.e., the variables to shoot with).
2) For a problem without air, use IFX1=0 and IFX2=0.
3) For a problem with air, single phase gas usually exists at the lower limit of the integration, ZL, and IFX1 applies there; two-phase conditions exist at the upper limit, ZU, and IFX2 applies there. When strong vapor pressure lowering causes two phase conditions to extend to ZL, boundary conditions should still be specified in terms of gas-phase variables (the program converts to two-phase variables internally). Because the range of variation of $P_a(z_L)$ is so large, IFX1=2 is usually preferable to IFX1=0.
4) The IFX1=1 and IFX2=1 options are provided for compatibility with TOUGH output. Our studies have shown little difference in convergence behavior between IFX1, IFX2=0 and IFX1, IFX2=1. Under certain conditions numerical accuracy is lost using IFX1=1 or IFX2=1. In such cases the code prints a warning message and stops.

2. Boundary Conditions

<u>QW0 QA0 QE0 V(1) V(3) V(3)</u>

FORMAT (6E10.4)

Flow rates at ZL ($r=0$ and $t=\infty$)

QW0 water flow rate Q_{w0} (kg/s/m) (nonzero values of QW0 are untested)

QA0 air flow rate Q_{a0} (kg/s/m) (nonzero values of QA0 are untested)

QE0 heat flow rate Q_{e0} (W/m) (if negative use IDEL=-1, untested)

State variables at ZU ($r=\infty$ and $t=0$)

Single-phase gas at ZU:

V(1) P_0 (Pa)

V(2) T_0 (°C)

V(3) P_{a0}, X^a_{g0}, or $\ln(P_{a0})$ for IFX1=0, 1, or 2, respectively (P_{a0} is in Pa; X^a_{g0} is dimensionless).

Single-phase liquid at ZU:

V(1) P_0 (Pa)

V(2) T_0 (°C)

V(3) P_{a0}, X^q_{l0}, or $\ln(P_{a0})$ for IFX1=0, 1, or 2, respectively (P_{a0} is in Pa; X^q_{l0} is dimensionless).

Two-phase at ZU:

V(1) P_0 (Pa)

V(2) S_{g0}

V(3) P_{a0}, X^a_{g0}, $\ln(P_{a0})$, or T_0 for IFX2=0 or 1, 2, or 3, respectively (P_{a0} is in Pa; X^q_{l0} is dimensionless).

Note: For a problem without air, set V(3)=0.

3. Material Properties

PERM PHI RHOR CR RKML RKMV COM EXPAN

FORMAT (8E10.4)

PERM	intrinsic permeability, k (m^2) (for effective-continuum representation of fractured/porous medium, matrix permeability is read here and fracture permeability is read in item 4)
PHI	initial porosity; porosity varies with compressibility (COM) and expansivity (EXPAN) (for effective-continuum representation of fractured/porous medium, matrix porosity is read here and fracture porosity is read in item 4)
RHOR	rock density (kg/m^3)
CR	rock heat capacity (J/kg K)
RKML	thermal conductivity of liquid-saturated rock (W/mK)
RKMV	thermal conductivity of gas-saturated rock (W/mK)
COM	rock compressibility (1/Pa) (should be nonzero for problems without air; suggest $\sim 10^{-8}$)
EXPAN	rock expansivity, constant (1/K)

Note: Thermal conductivity varies with the square root of liquid saturation between the limits of RKML and RKMV.

TORTX DIFF0 TEXP BETA BKNUD

FORMAT (5E10.4)

TORTX	gas-phase tortuosity
DIFF0	strength parameter of binary diffusion coefficient (m^2/s)
TEXP	parameter for temperature dependence of binary diffusion (default 1.8)
BETA	enhanced vapor diffusion parameter BETA = 0: vapor diffusion coefficient=air diffusion coefficient; BETA > 0: BETA=TORTX*PHI*S_g in vapor diffusion coefficient
BKNUD	Klinkenberg b parameter for Knudsen diffusion (Pa)

Note: TORTX, DIFF0, and TEXP follow the TOUGH usage. TORTX and DIFF0 must be nonzero if a single-phase gas zone exists.

4. Characteristic Curves

IRP RP(1) RP(2) RP(3) RP(4) RP(5) RP(6) RP(7)

FORMAT (I5,5X,7E10.4)

IRP flag to identify relative permeability function

(RP(I),I=1,7) parameters of relative permeability function (see Table 1)

ICP CP(1) CP(2) CP(3) CP(4) CP(5) CP(6) CP(7)

FORMAT (I5,5X,7E10.4)

ICP flag to identify capillary pressure function

(CP(I),I=1,7) parameters of capillary pressure function (see Table 2)

Note: IRP=1-8, ICP=1-7 call the same functions as used in TOUGH.

Table 1. Overview of the parameters for relative permeability functions. For more details on IRP=1-8 see the TOUGH users guide [*Pruess*, 1987]. For more details on IRP=9-12 see below.

IRP	Identifier	RP(1)	RP(2)	RP(3)	RP(4)	RP(5)	RP(6)	RP(7)
1	linear	S_{lr}	S_{sr}	S_{ls}	S_{ss}			
2	$k_{rl}=S_l^n$, $k_{rg}=1$	n						
3	Corey	S_{lr}	S_{sr}					
4	Grant	S_{lr}	S_{sr}					
5	$k_{rl}=k_{rg}=1$							
6	Fatt & Klickoff	S_{lr}						
7	van Genuchten with $k_{rg}=1-k_{rl}$	λ	S_{lr}	S_{ls}				
8	Verma et al.	S_{lr}	S_{ls}	1.259	-1.7615	0.5089		
9	Eff. continuum, constant k_{rg}	λ	S_{lr}	S_{ls}	k_{rg}			
10	Eff. continuum, constant k_{rg}, k_{rl}	k_{rg}	k_{rl}					
11	Eff. continuum, seq. sat. model	λ	S_{lr}	S_{ls}	V_f	k_f	ϕ_f	
12	Eff. continuum, curve-fit	$\hat{k}_{th}$	$\hat{S}_{lr}$	S_{ls}	V_f	k_f	ϕ_f	$\hat{\varepsilon}$

Notation

S_{lr} – irreducible liquid saturation in relative permeability
S_{sr} – irreducible gas saturation in relative permeability
S_{ls} – liquid saturation at which $k_{rl}=1$
S_{ss} – gas saturation at which $k_{rg}=1$
λ – parameter in van Genuchten formulation
V_f – fracture volume (fraction of total volume)
k_f, ϕ_f – fracture intrinsic permeability (m^2) and porosity
$\hat{k}_{th}$, $\hat{S}_{lr}$, $\hat{\varepsilon}$ – fitting parameters for IRP=12 (see Figure 2)

Effective-Continuum IRP choices (not available in TOUGH)

IRP=9 *van Genuchten* [1980] formulation for k_{rl}; constant value of k_{rg}, may be large (>>1) to represent enhanced gas-phase flow in fractures. Parameters S_{lr} and S_{ls} relate to matrix saturation only.

IRP=10 Constant values of k_{rl} and k_{rg}, may be large (>>1) to represent enhanced flow of both liquid and gas phases in fractures.

IRP=11 Sequential-saturation model: uses *van Genuchten* [1980] formulation for matrix, and $k_{rlf} = S_{lf}$ for fractures. Parameters S_{lr} and S_{ls} relate to matrix saturation only.

IRP=12 Creates an effective $\tilde{k}_{rl}$ using the parameters shown in Figure 2; then takes $\tilde{k}_{rg} = 1 - \tilde{k}_{rl}$. This option is useful for curve-fitting to given k_{rl} curves that do not have a simple analytical form, such as those calculated iteratively in the concurrent-saturation model, or those based on experimental measurements.

Table 2. Overview of the parameters for capillary pressure functions. For more details on ICP=1-7 see the TOUGH users guide [*Pruess*, 1987]. For more details on ICP=8 see below.

ICP	Identifier	CP(1)	CP(2)	CP(3)	CP(4)	CP(5)	CP(6)
1	linear	P_{max}	S_{lr}	$S_{ls} = 1$			
2	Pickens	P_{c0}	S_{lr}	S_{l0}	x		
3	Trust	P_{c0}	S_{lr}	η	P_e	P_{max}	
4	Milly	S_{lr}					
5	(none)						
6	Leverett		S_{lr}	T_0			
7	van Genuchten	λ	S_{lr}	$1/P_{c0}$	P_{max}	$S_{ls} = 1$	
8	Eff. continuum (IRP=11, 12)	λ	S_{lr}	$1/P_{c0}$	P_{max}	$S_{ls} = 1$	δ_s

Notation

S_{lr} – irreducible liquid saturation in capillary pressure
S_{ls} – liquid saturation at which $P_c = 0$, must be 1
P_{c0} – capillary pressure reference strength (Pa)
P_{max} – maximum strength of capillary pressure (Pa)
S_{l0}, x – parameters in Pickens formulation
η, P_e – parameters in Trust formulation (P_e is in Pa)
T_0 – reference temperature at which to calculate P_c in Leverett formulation (if blank, P_c depends on temperature through steam-table temperature dependence of surface tension)
λ – parameter in van Genuchten formulation
δ_s – parameter in effective continuum formulation

Effective-Continuum ICP choice (not available in TOUGH)

ICP=8 To be used with IRP=11 or IRP=12 only. Uses the *van Genuchten* [1980] formulation for matrix and a linear variation of P_c in the fractures. At the transition between matrix and fracture flow, $P_{cf}(S_{lf}) = P_{cm}(S_{lm})$, with $S_{lf} = 0$ and $S_{lm} = 1 - \delta_s$. With a suitable choice of δ_s, this form also may be used to match the iteratively-calculated P_c curve of the concurrent-saturation model.

5. Integration Parameters

INTMIN INTMAX

FORMAT (2E10.4)

INTMIN lower limit of integration

INTMAX upper limit of integration

Notes:

1) If INTMIN is positive, INTMIN and INTMAX are integration limits in terms of the variable $\eta = r/\sqrt{t}$. If INTMIN is negative, INTMIN and INTMAX are limits in terms of the variable $z = \ln(\eta)$. In either case, the integration variable used in SIMSOL is z.

2) For shooting to work, all flow rates should be constant at INTMIN ($dQ/dz = 0$) and zero at INTMAX. Simple analytical solutions may be used to provide rough values for INTMIN and INTMAX [e.g., *Doughty and Pruess*, 1990, p. 1211]. Alternatively, a few preshots may be used to determine appropriate values of INTMIN and INTMAX.

EPS HMIN DV0 F0 TINY

FORMAT (5E10.4)

EPS accuracy criterion for step-size growth (default 10^{-5})

HMIN minimum allowed step size (default SMALL, see below)

DV0 relative convergence criterion for V at ZL (default 0.01)

F0 relative convergence criterion for V at ZU (default 0.01)

TINY very small quantity used as numerical "zero" (default value calculated internally as the smallest number such that 1 + TINY > 1; a user-input value of TINY cannot be less than the default) Program calculates SMALL= $\sqrt{\text{TINY}}$ for use in many contexts. As derived, calculated differences greater than SMALL have at least half significant digits.

QWSCALE QESCALE PSCALE TSCALE (or SSCALE) QASCALE PASCALE

FORMAT (6E10.4)

Scaling factors to determine acceptance of an integration step. For most problem setting all scaling factors to zero works fine. Collectively, the scaling factors make up a six-entry vector YSCALE. A nonzero value of YSCALE is useful for problems in which there is a component of Y for which both Y and DYDX are near zero during some part of the integration. If an entry of YSCALE is −1 the following default value is used: QWSCALE=$Q_{e0}/2\times10^6$, QESCALE=Q_{e0}, PSCALE=P_0, TSCALE or SSCALE = 1, QASCALE=$Q_{e0}/2\times10^9$, PASCALE = max(1, P_{a0}). The rationale for these default values is very heuristic and detailed testing has not been done. A step is accepted if (Y1-Y2)/max(Y2+H*DYDX,YSCALE) < EPS, where Y1 and Y2 are 6-entry vectors containing the primary variables after a whole step and two-half steps, respectively; DYDX is the vector of derivatives of the primary variables with respect to the integration variable; H is the integration step length; and EPS is the accuracy criterion read in above.

6. Initial Guesses for Missing Boundary Conditions at ZL and Newton-Raphson Increments

V(1) DELV(1) V(2) DELV(2) V(3) DELV(3)

FORMAT (6E10.4)

(V(I),I=1,3) Initial guesses for shooting variables at ZL ($r = 0$, $t = \infty$)

Single-phase gas at ZL:

V(1) = P_0 (Pa)

V(2) = T_0 (°C)

V(3) = P_{a0}, X^a_{g0}, or $\ln(P_{a0})$ for IFX1=0, 1, or 2, respectively (P_{a0} is in Pa, x^a_{l0} is dimensionless).

Single-phase liquid at ZL:

V(1) = P_0 (Pa)

V(2) = T_0 (°C)

V(3) = P_{a0}, X^a_{l0}, or $\ln(P_a)$ for IFX1=0, 1, or 2, respectively (P_{a0} is in Pa, X^a_{l0} is dimensionless).

Two-phase at ZL:

V(1) = P_0 (Pa)

V(2) = S_{g0}

V(3) = P_{a0}, X^a_{g0}, $\ln(P_{a0})$, or T_0 for IFX1=0, 1, 2, or 3, respectively (P_{a0} is in Pa, X^a_{l0} is dimensionless).

(DELV(I),I=1,3) Increment for Newton Raphson iterations. If zero, calculated internally each iteration to be $\sqrt{\text{EPS}}$ times the current value of V(I).

Notes:

1) For a problem without air, set V(3)=0. Conversely for a problem with air V(3) must be nonzero, although it may be quite small.

2) When vapor-pressure-lowering is on (IVPL=1) specify initial guesses at ZL as though it were off (IVPL=0 or 2); code will calculate modified guesses to account for vapor-pressure-lowering.

III. RUNNING SIMSOL

1. Files Used

1. INPUT — As described above; program skips one header line for each data line in input file (see examples in Section IV). Referred to in source code as Unit 5.
2. OUTPUT — Subset of output printed to screen; shows input, iteration behavior, convergence, costs (see examples in Section IV). Referred to in source code as Unit 8.
3. PLOT — Profiles of variables as a function of z, for post-process plotting (Table 3 describes the contents of PLOT; see examples in Section IV). Referred to in source code as Unit 7.

2. Batch Mode Versus Interactive Mode

The usual way to run SIMSOL is in interactive mode (IBAT=0 in input file, item 1). In interactive mode, the user starts out in the 'Preshoot Section', where initial guesses for variables at the lower limit of integration (V(1), V(2), and V(3)), the limits of integration (ZL and ZU), and the accuracy-controlling parameter EPS are entered from the keyboard and individual numerical integrations are done. A value of zero for a parameter indicates that the previous value should be used. This section is useful for gaining insight into the general physical behavior of the problem at hand.

To exit Preshoot Section, the user enters V(1)=-1, and any values for V(2) and V(3). The user may then enter the 'Shooting Section' or quit. In the Shooting Section, Newton-Raphson iteration is carried out. At each iteration, a main integration and three integrations using incremented values of primary variables at the lower limit of integration are done. The program then solves the resulting system of linear equations for updated values of the primary variables at the lower limit of integration. The user enters the Shooting Section in 'Interactive Mode', with the option of modifying the values of the primary variables at the lower limit of integration after each iteration (that is, overriding the results of the Newton-Raphson iteration). Also, after each iteration, the user has the option of switching to 'Batch Mode' or quitting. In Batch Mode, shooting proceeds with no additional input from the user.

If IBAT=1, the program skips Preshoot Section and carries out the shooting algorithm in Batch Mode, with no keyboard input from the user. The flow chart in Figure 1 illustrates these options.

3. Screen Output

The basic screen output during a SIMSOL run is very similar to the information printed in the OUTPUT file. In addition, in interactive mode (IBAT=0) the user has the option of choosing two additional kinds of output by responding to prompts given at the start of the run.

1) Extra output during numerical integrations. At every 50 steps during the numerical integration a short status report of the progress of the integration is printed to the screen. In addition, if the integration step needs to be greatly decreased (as often happens at phase-change points) it is reported. For slow computers, or long integrations, this output can reassure the user that the program is continuing to run.

2) Interactive graphics output. This requires a graphics terminal and a subroutine SIMPLOT that interfaces correctly with the user's graphics library. Two subroutines are provided with the source code: one that works on a LBL VAX 6420 and one that works on a Cray 2 at the NERSC; both are designed to be used with a Tektronix-type graphics terminal. Each version is annotated to provide guidelines for customizing the graphical interface to the user's own system. The subroutine SIMPLOT generates simple plots of T, P, S_l, and X_g^a profiles during Preshooting. These profiles are very helpful in determining improved guesses for missing boundary conditions.

4. Post-Processing Graphical Output

In addition to writing general information to the file OUTPUT, SIMSOL creates a file called PLOT which contains data in a form suitable for graphical post-processing. Each line of the file PLOT is of the form:

INFO LABEL Z VAR1(Z) VAR2(Z) VAR3(Z) VAR4(Z) VAR5(Z) NSTP IPH IERR

FORMAT(2A5,6E10.4,I5,2I2)

INFO — if the numerical integration of the ordinary differential equations cannot be carried out to ZU for some reason, INFO is 'p-ode' (partial integration); for successful pre-shots (in which the integration can be carried out to ZU), INFO is 'f-ode' (full integration); for successful shots INFO is blank.

LABEL — identifies which variables are printed on the line (see Table 3)

Z — value of the integration variable; $z = \ln(\eta) = \ln(r/\sqrt{t})$

VAR1(Z)...VAR5(Z) — value of variables at z (see Table 3 and notes)

NSTP — index number of the integration step (all steps are listed if NZ=0, see input description, item 1)

IPH — phase flag: 1=gas phase, 3=two-phase, 4=liquid phase

IERR — variable controlling convergence: 1=Q_w, 2= Q_e, 3=P, 4=T (single phase) or S (two-phase), 5=Q_a, 6=P_a.

Table 3. Contents of the file PLOT.

LABEL	VAR1	VAR2	VAR3	VAR4	VAR5
aa*ij* or aa*ij*0	Q_w	Q_e	P	T	Q_a
bb*ij* or bb*ij*0	P_a or $\ln(P_a)$‡	S_g	Q_g	Q_l	X_g^a
ee*ij* or ee*ij*0	DYP(1)	DYP(2)	DYP(3)	DYP(4)	DYP(5)
ffi*j* or ffi*j*0	DYP(6)	HP	P_c	dP_c/dS	dT_{sat}/dS

‡Depends on the value of ILOG, see input description, item 1

Notes:

1) The first form of LABEL shown identifies the *ij*TH preshot; the second form identifies the *ij*TH shot, where *ij* is a two-digit number.
2) The subscripts g, l, w, a, and e indicate gas, liquid, water, air, and energy, respectively.
3) DYP are the derivatives used in the numerical integration.
4) HP is the integration step length.
5) In the OUTPUT files, flow rate terms are normalized by a factor of 2π, as they appear in the calculations; in the PLOT file the unnormalized values are given.
6) Units: mass flow rate – kg/s/m, heat flow rate – W/m, pressure – bars (Pa/10^5), temperature – °C.

5. Machine Dependencies

The file README.TXT, which is distributed along with the source code, includes specific instructions for compiling and running SIMSOL on several computers. As noted above, use of interactive graphics is very dependent on the system being used. Here some general comments relating to more fundamental issues of machine dependency are made.

SIMSOL is written entirely in FORTRAN. It was developed on a Cray 2 at the NERSC at LLNL, which is a 64 bit machine, using single precision. It has also been tested on a VAX 6420, a 32 bit machine, using the VMS operating system. To run on a 32 bit machine, double precision must be used. The switch to double precision can be accomplished easily on some 32 bit computers merely by removing the 'C' from column one of the line

```
C     IMPLICIT DOUBLE PRECISION
```

which appears in every program unit (i.e., main program, all subroutines and functions). A number of real constants are specified in the source code, and some compilers (e.g. VMS Fortran on the LBL VAXes) automatically convert them to double precision when the IMPLICIT DOUBLE PRECISION statement is used. If this is not the case, then these constants must be converted from F or E format to D format in the source code in order to invoke double precision properly.

When running on the NERSC Cray three system routines are called; these calls must be replaced or eliminated when running on another machine.

LINK – initializes input and output files

EMPTY (LUN) – flushes buffers after printing to Unit LUN

SECOND (ELT) – returns ELT, current CPU-time, at various stages

The simplest way to eliminate the calls is to include dummy subroutines in the source code (this has been done for LINK and EMPTY in the VAX version of SIMSOL that is being distributed). If the functionality of the calls is needed but the system routine name or method of calling differs from that of the NERSC Cray, the user may call the appropriate system routines from routines called LINK, EMPTY, or SECOND, and thus avoid making numerous changes throughout the SIMSOL source code (this has been done for SECOND in the VAX version of SIMSOL that is being distributed).

An EMPTY-type call is unecessary if print buffers are automatically flushed after printing. Additionally, a LINK-type call is unecessary if input/output file initialization is done outside the

code. Using VMS on a VAX, for example, one would define

```
FOR005   INPUT
FOR008   OUTPUT
FOR007   PLOT
```

before running SIMSOL. These definitions can be included in a command file, but then provisions must be made to allow input to be read from the keyboard, and output to be sent to the screen (see the example SIM.COM included with the source code).

On some computers it may be necessary to add SAVE statements to each subroutine and function, to ensure that variable values are preserved between successive calls. The use of SAVE statements, while formally necessary in standard Fortran, is not needed for many computers, in particular the Crays and VAXes on which SIMSOL has been run.

6. Suggested Strategies

1) When possible, run a new problem as a perturbation of an already solved problem, so reasonable initial guesses for some or all V's will be available.

2) It may be beneficial to run a version of the problem without air first. Use the figures from LBL-26057 to provide initial guesses for V and insight into the general physical behavior of the system. The presence of air generally decreases heat-pipe length. Create an 'air table', by doing a sequence of preshots with increasing amounts of air. Based on the best entry in the air table, do one shot. While the resulting 'improved' value of P_{aL} may be physically meaningless (e.g., negative), the new values of P_L and T_L are often good, and can provide the basis for an improved air table.

3) Vapor pressure lowering usually just has a small, localized effect on the saturation profile. Run without it first. With vapor pressure lowering, dP_c/dS must be nonzero when $S_l < S_{lr}$ (e.g., ICP=1 with a nonzero value of S_{lr} produces a constant value of $P_c = P_{\max}$ for $S_l < S_{lr}$, and the code will not work). Using $S_{lr} = 0$ in the capillary pressure function is usually a good idea, even if S_{lr} is nonzero in the relative permeability function. For strong vapor pressure lowering, the temperature can be very large in the two-phase zone. To help stay within the range of the liquid equation of state, the option of using the 'unlowered' vapor pressure is being developed (IVPL=-1), but it does not work now. If temperatures are too large, try a bigger value of ZL.

4) Use larger values of EPS ($\sim 10^{-3}$) during preshooting to get a rough idea of general physical behavior quickly. Before shooting, rerun the best case with a 10 times smaller value of EPS. Repeat until the results are not significantly different. Shooting may not converge if the value of EPS is too big. For some well behaved problems, it may be possible to do 'rough shooting' with a large value of EPS, then decrease EPS as the actual solution is neared.

IV. SAMPLE PROBLEMS

INPUT and OUTPUT files and partial PLOT files are given for six sample problems. The calculations were made using a Cray 2 at NERSC. Graphical presentation of the plot-file data appears in *Doughty and Pruess* [1991]. The six sample problems are:

1. Moderate permeability medium, no air (Figure 1, DP91)
2. Moderate permeability medium, air and water (Figure 1, DP91)
3. Low permeability medium, vapor pressure lowering (Figure 5, DP91)
4. Effective continuum, sequential-saturation model (Figure 8, DP91)
5. Effective continuum, curve-fit to concurrent-saturation model (Figure 10, DP91)
6. Moderate permeability medium, enhanced vapor diffusion (Figure 11, DP91)

Problems 1, 3, 4, and 5 use the correct values of V at ZL, so no shooting is done. Problems 2 and 6 illustrate the shooting method. In problem 2 a sequence of preshooting and shooting is illustrated by adding air to the problem without air (problem 1). In problem 6 enhanced vapor diffusion (BETA=1) is added to the air and water problem (problem 2); the overall effect is small enough so that preshooting is not needed and shooting can be done immediately using the values of V at ZL for problem 2. Extensive descriptions of the physical processes taking place in the sample problems may be found in *Doughty and Pruess* [1991].

Problem 1: Problem without air (input, output, and partial plot files shown)

For a problem without air IFX1 and IFX2 must be zero, and state-variable boundary conditions are specified as pressure and temperature. For this example, the intrinsic permeability is moderately large (PERM = 20×10^{-15}) and the van Genuchten characteristic curves (IRP=ICP=7) are used (see input file). Using a convergence criterion EPS = 10^{-4}, 142 steps are needed for the numerical integration (see output file). To check the accuracy of the algorithm, the integration can be done using a smaller value of EPS (results not shown). For EPS = 10^{-5}, 178 steps are needed, but the results do not change, indicating that EPS = 10^{-4} is sufficient for this problem. In general, longer heat pipes may require smaller values of EPS.

Sample problem 1 input file.

```
 ifx1 ifx2   nz ibat ivpl ilog idel
    0    0  200    0    0    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    18.        0.
perm       phi        rhor       cr         rkml       rkmv       com        expan
20.   e-15 0.10       2550.      800.       2.         2.         1.     e-7 0.
tortx      diff0      texp       beta       bknud
0.50       2.6   e-05 1.   e-10 0.         0.0     e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
    7      0.45       9.6   e-04 1.0
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    7      0.45       1.0   e-03 8.   e-05 5.0  e+08 1.0
intmin     intmax
-11.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.   e-11 1.    e-2 1.    e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
123400.    0.0        232.6      0.0        0.0        0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.200e-13  phi0= 0.100e+00  rhor= 0.255e+04    cr= 0.800e+03
 rkml= 0.200e+01  rkmv= 0.200e+01   com= 0.100e-06 expan= 0.
tortx= 0.500e+00 diff0= 0.260e-04  texp= 0.100e-09
 beta= 0.        bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
  7  0.4500e+00 0.9600e-03 0.1000e+01 0.          0.          0.
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  7  0.4500e+00 0.1000e-02 0.8000e-04 0.5000e+09 0.1000e+01 0.

   Slr=0.9600e-03 Sltest=0.1264e-02   krl=0.8350e-18   krg=0.1000e+01
   pc2=-.1306e+13  denom=0.1090e-05

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           T0           Pa0
       0.100000e+06 0.180000e+02 0.
       S0           Xga          Xla
       0.           0.           0.

Integration Parameters
----------------------
etamin=0.1670e-04 etamax=0.6738e-02     zL=  -11.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.             Qe=0.             P=0.         T or S=0.
    Qa=0.             Pa=0.
 nzsav= 200        dzsav=0.3000e-01   ibat=0 ifx1=0 ifx2=0 ivpl= 0 idel= 1

 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1234e+06  0.2326e+03  0.
 new  v=0.          0.          0.
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1234e+06  T= 232.6000
Sg=0.1000e+01 Pa=0.         Xg=0.         Xl=0.
        ODEINT done,    zU=  -5.000, iph=4  , nok= 86, nbad= 56
Qw=0.3945e-05 Qe=0.2983e+00 Qa=0.          P=0.1000e+06  T=  17.9786
Sg=0.         Pa=0.         Xg=0.         Xl=0.
Converged

ith= 2
 old  v=0.1234e+06  0.2326e+03  0.
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.1714e+01 seconds

 _________
|         |
|  Shoot  |
|_________|

-----------------------------------------------------------------------
Starting values for shot  1
   v=0.1234e+06  0.2326e+03  0.
delv=0.1234e+04  0.2326e+01  0.          eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
1
Stop
```

Sample problem 1 output file.

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
f-ode aa 1	-11.000000.		667.6700	1.23400	232.60000.		1	1	0
f-ode aa 1	-10.968450.	1634e-12	667.6672	1.23400	230.92380.		3	1	1
f-ode aa 1	-10.875680.	7159e-12	667.6579	1.23400	225.99480.		4	1	1
f-ode aa 1	-10.565240.	3666e-11	667.6108	1.23400	209.50160.		5	1	1
f-ode aa 1	-10.274620.	9062e-11	667.5305	1.23400	194.06270.		6	1	1
f-ode aa 1	-9.965850.	2033e-10	667.3748	1.23400	177.66250.		7	1	1
f-ode aa 1	-9.650570.	4365e-10	667.0780	1.23400	160.92190.		8	1	1
f-ode aa 1	-9.333390.	9184e-10	666.5162	1.23400	144.09050.		9	1	1
f-ode aa 1	-9.016980.	1912e-09	665.4616	1.23400	127.32060.		10	1	1
f-ode aa 1	-8.702740.	3957e-09	663.4987	1.23400	110.70180.		11	1	1
f-ode aa 1	-8.606360.	4947e-09	662.6062	1.23400	105.61600.		0	1	0
f-ode aa 1	-8.606360.	4947e-09	662.6062	1.23400	105.61600.		12	3	1
f-ode aa 1	-8.566940.	3798e-05	664.2127	1.22054	105.29850.		32	3	1
f-ode aa 1	-8.517860.	4859e-05	664.5819	1.20364	104.89550.		34	3	1
f-ode aa 1	-8.473340.	5620e-05	664.8149	1.18814	104.52200.		35	3	4
f-ode aa 1	-8.404340.	6741e-05	665.1222	1.16374	103.92560.		36	3	4
f-ode aa 1	-8.291780.	8809e-05	665.6330	1.12257	102.89540.		37	3	1
f-ode aa 1	-8.194670.	1114e-04	666.1696	1.08450	101.91460.		38	3	1
f-ode aa 1	-8.125540.	1321e-04	666.5902	1.05377	101.10190.		40	3	4
f-ode aa 1	-8.091980.	1430e-04	666.7481	1.03591	100.62070.		42	3	4
f-ode aa 1	-8.060660.	1524e-04	666.7175	1.01316	99.99740.		47	3	4
f-ode aa 1	-8.053160.	1536e-04	666.5887	1.00403	99.74400.		0	3	0
f-ode aa 1	-8.053160.	1536e-04	666.5887	1.00403	99.74400.		101	4	4
f-ode aa 1	-8.014950.	1540e-04	665.1245	1.00401	97.73880.		116	4	2
f-ode aa 1	-7.900330.	1556e-04	660.0142	1.00397	91.75060.		117	4	2
f-ode aa 1	-7.441850.	1658e-04	623.5290	1.00376	68.43620.		118	4	2
f-ode aa 1	-7.007510.	1830e-04	546.4430	1.00346	48.19950.		119	4	1
f-ode aa 1	-6.637870.	2038e-04	425.6522	1.00309	33.85390.		120	4	1
f-ode aa 1	-6.236180.	2277e-04	235.9420	1.00251	23.25250.		121	4	2
f-ode aa 1	-6.109810.	2341e-04	173.6241	1.00229	21.21760.		122	4	2
f-ode aa 1	-5.987250.	2392e-04	118.7172	1.00206	19.81810.		123	4	2
f-ode aa 1	-5.886510.	2425e-04	80.5344	1.00187	19.04000.		124	4	2
f-ode aa 1	-5.802280.	2447e-04	54.7115	1.00170	18.60300.		125	4	2
f-ode aa 1	-5.728910.	2461e-04	37.0892	1.00155	18.34830.		126	4	2
f-ode aa 1	-5.664460.	2471e-04	25.2665	1.00141	18.19950.		127	4	2
f-ode aa 1	-5.607230.	2477e-04	17.3963	1.00130	18.11180.		128	4	2
f-ode aa 1	-5.555170.	2481e-04	12.1122	1.00119	18.05910.		129	4	2
f-ode aa 1	-5.503730.	2483e-04	8.3636	1.00108	18.02530.		130	4	2
f-ode aa 1	-5.456240.	2485e-04	5.9516	1.00098	18.00560.		131	4	2
f-ode aa 1	-5.412850.	2485e-04	4.4361	1.00089	17.99440.		132	4	2
f-ode aa 1	-5.371950.	2486e-04	3.4652	1.00081	17.98770.		133	4	2
f-ode aa 1	-5.333510.	2485e-04	2.8542	1.00073	17.98390.		134	4	2
f-ode aa 1	-5.296830.	2485e-04	2.4698	1.00065	17.98160.		135	4	2
f-ode aa 1	-5.261070.	2485e-04	2.2278	1.00058	17.98030.		136	4	2
f-ode aa 1	-5.225400.	2484e-04	2.0766	1.00050	17.97950.		137	4	2
f-ode aa 1	-5.189390.	2484e-04	1.9847	1.00043	17.97910.		138	4	2
f-ode aa 1	-5.152720.	2483e-04	1.9310	1.00035	17.97890.		139	4	2
f-ode aa 1	-5.114720.	2482e-04	1.9010	1.00027	17.97870.		140	4	2
f-ode aa 1	-5.074650.	2481e-04	1.8850	1.00019	17.97870.		141	4	2
f-ode aa 1	-5.031770.	2480e-04	1.8770	1.00010	17.97860.		142	4	2
f-ode aa 1	-5.000000.	2479e-04	1.8740	1.00003	17.97860.		143	4	2

Sample problem 1 plot file (partial).

Label	z	P_a (bars)	S_g	Q_g (kg/s/m)	Q_l (kg/s/m)	X_g^a	NSTP	IPH	IERR
f-ode bb 1	-11.000000.		0.1000e+010.	0.	0.		1	1	0
f-ode bb 1	-10.968450.		0.1000e+010.	1634e-120.	0.		3	1	1
f-ode bb 1	-10.875680.		0.1000e+010.	7159e-120.	0.		4	1	1
f-ode bb 1	-10.565240.		0.1000e+010.	3666e-110.	0.		5	1	1
f-ode bb 1	-10.274620.		0.1000e+010.	9062e-110.	0.		6	1	1
f-ode bb 1	-9.965850.		0.1000e+010.	2033e-100.	0.		7	1	1
f-ode bb 1	-9.650570.		0.1000e+010.	4365e-100.	0.		8	1	1
f-ode bb 1	-9.333390.		0.1000e+010.	9184e-100.	0.		9	1	1
f-ode bb 1	-9.016980.		0.1000e+010.	1912e-090.	0.		10	1	1
f-ode bb 1	-8.702740.		0.1000e+010.	3957e-090.	0.		11	1	1
f-ode bb 1	-8.606360.		0.1000e+010.	4947e-090.	0.		0	1	0
f-ode bb 1	-8.606360.		0.9987e+000.	2508e-03-	.2508e-030.		12	3	1
f-ode bb 1	-8.566940.		0.6269e+000.	2499e-03-	.2461e-030.		32	3	1
f-ode bb 1	-8.517860.		0.5337e+000.	2487e-03-	.2439e-030.		34	3	1
f-ode bb 1	-8.473340.		0.4730e+000.	2476e-03-	.2419e-030.		35	3	4
f-ode bb 1	-8.404340.		0.3933e+000.	2455e-03-	.2387e-030.		36	3	4
f-ode bb 1	-8.291780.		0.2711e+000.	2408e-03-	.2320e-030.		37	3	1
f-ode bb 1	-8.194670.		0.1597e+000.	2334e-03-	.2222e-030.		38	3	1
f-ode bb 1	-8.125540.		0.7581e-010.	2203e-03-	.2071e-030.		40	3	4
f-ode bb 1	-8.091980.		0.3582e-010.	2036e-03-	.1893e-030.		42	3	4
f-ode bb 1	-8.060660.		0.3855e-020.	1387e-03-	.1235e-030.		47	3	4
f-ode bb 1	-8.053160.		0.5624e-070.	1817e-050.	1354e-040.		0	3	0
f-ode bb 1	-8.053160.		0.	0.	0.1536e-040.		101	4	4
f-ode bb 1	-8.014950.		0.	0.	0.1540e-040.		116	4	2
f-ode bb 1	-7.900330.		0.	0.	0.1556e-040.		117	4	2
f-ode bb 1	-7.441850.		0.	0.	0.1658e-040.		118	4	2
f-ode bb 1	-7.007510.		0.	0.	0.1830e-040.		119	4	1
f-ode bb 1	-6.637870.		0.	0.	0.2038e-040.		120	4	1
f-ode bb 1	-6.236180.		0.	0.	0.2277e-040.		121	4	2
f-ode bb 1	-6.109810.		0.	0.	0.2341e-040.		122	4	2
f-ode bb 1	-5.987250.		0.	0.	0.2392e-040.		123	4	2
f-ode bb 1	-5.886510.		0.	0.	0.2425e-040.		124	4	2
f-ode bb 1	-5.802280.		0.	0.	0.2447e-040.		125	4	2
f-ode bb 1	-5.728910.		0.	0.	0.2461e-040.		126	4	2
f-ode bb 1	-5.664460.		0.	0.	0.2471e-040.		127	4	2
f-ode bb 1	-5.607230.		0.	0.	0.2477e-040.		128	4	2
f-ode bb 1	-5.555170.		0.	0.	0.2481e-040.		129	4	2
f-ode bb 1	-5.503730.		0.	0.	0.2483e-040.		130	4	2
f-ode bb 1	-5.456240.		0.	0.	0.2485e-040.		131	4	2
f-ode bb 1	-5.412850.		0.	0.	0.2485e-040.		132	4	2
f-ode bb 1	-5.371950.		0.	0.	0.2486e-040.		133	4	2
f-ode bb 1	-5.333510.		0.	0.	0.2485e-040.		134	4	2
f-ode bb 1	-5.296830.		0.	0.	0.2485e-040.		135	4	2
f-ode bb 1	-5.261070.		0.	0.	0.2485e-040.		136	4	2
f-ode bb 1	-5.225400.		0.	0.	0.2484e-040.		137	4	2
f-ode bb 1	-5.189390.		0.	0.	0.2484e-040.		138	4	2
f-ode bb 1	-5.152720.		0.	0.	0.2483e-040.		139	4	2
f-ode bb 1	-5.114720.		0.	0.	0.2482e-040.		140	4	2
f-ode bb 1	-5.074650.		0.	0.	0.2481e-040.		141	4	2
f-ode bb 1	-5.031770.		0.	0.	0.2480e-040.		142	4	2
f-ode bb 1	-5.000000.		0.	0.	0.2479e-040.		143	4	2

Sample problem 1 plot file (partial).

Problem 2: Example of preshooting/shooting sequence (input, output, and partial plot files shown)

Air is added to problem 1 by specifying two-phase boundary conditions at ZU: IFX2=3, P_0 = 1 bar, S_{g0} = 0.2, T_0 = 18°C, rather than single-phase liquid conditions: IXF1=0, P_0 = 1 bar, T_0 = 18°C, P_{a0} = 0 (compare problem 1 and problem 2 input files). This requires that a nonzero value of P_a be specified at ZL (input item 6, note 1). Experience has shown that the value of $P_a(z_L) \equiv P_{aL}$ depends strongly on the strength and length of the heat pipe, making it difficult to determine a reasonable initial guess for shooting. Therefore preshooting is done, to ascertain the overall effect of adding air.

The first preshot (see output file, ith=1) uses the initial values of V(1) = $P(z_L) \equiv P_L$ = 1.234 bars and V(2) = $T(z_L) \equiv T_L$ = 232.6°C from the problem without air, and adds a small amount of air: V(3) = $\ln(P_{aL})$ = −100 (note that IFX1=2 so that V(3) is $\ln(P_{aL})$ rather than P_{aL}). The resulting values of $P(z_U) \equiv P_U$ = 1.038 bars and $T(z_U) \equiv T_U$ = 16.63°C are not too different from P_0 = 1 bar and T_0 = 18°C, but the value of $S_g(z_U) \equiv S_U$ = 0.052 is much smaller than S_{g0} = 0.2. Usually this combination of results indicates that more air is needed, so another preshot is tried (ith=2), this time specifying V(3) = −20. The numerical integration is unable to finish, as the vapor partial pressure (P_v, called Ps in SIMSOL) becomes so small that the temperature goes out of bounds in the equation of state package for liquid/gaseous water (T < 3°C). Vapor partial pressure is calculated from $P = P_v + P_a$, so P_v can be too small if P is too small or if P_a is too large. The output indicates that P = 1.135 bars just before the integration stops at z = −6.18, which is greater than P_0, hence not too small. Thus V(3) = $\ln(P_{aL})$ = −20 is likely to be too large. Another preshot is tried (ith=3), using V(3) = −50. The resulting values of P_U = 1.08 bars, S_U = 0.179, and T_U = 12.63°C are all reasonably close to the specified conditions P_0 = 1 bar, S_{g0} = 0.2, and T_0 = 18°C, so shooting is commenced.

The values of V used for the ith=3 preshot could be used as is for the first shot, but they can also be modified slightly ('nudged') to try to get closer to the specified boundary conditions at ZU (i.e., $P_U > P_0$ so V(1) is decreased slightly; $T_U < T_0$ and $S_U < S_{g0}$ so V(2) and V(3) are increased slightly). Using 'nudged' values for V, the first shot (is=1) gives P_U = 0.98 bars, S_U = 0.19, and T_U = 16.7°C. The second shot (is=2) takes V(1) = 1.15 bars, V(2) = 239.5°C, and V(3) = −43.7, and converges, with P_U, S_U, and T_U matching P_0, S_{g0}, and T_0 within the required accuracy F0 = 0.01.

If the values of V from the ith=3 preshot are used without 'nudging' shooting is still successful (results not shown), but three shots are needed to converge. On the other hand, shooting from the ith=1 preshot is not successful (results not shown), as the Newton-Raphson algorithm calculates V(1) = 1.14 bars, V(2) = 239.4°C, and V(3) = 28.97 ($P_{aL} = e^{28.97}$ bars) for the second shot. Although this value of V(3) is physically meaningless, and totally unusable since it makes $P_a \gg P$, the values for V(1) and V(2) are quite close to the converged values. Thus even unsuccessful shots may provide useful information for further preshooting or shooting.

Sample problem 2 input file.

```
 ifx1 ifx2   nz ibat ivpl ilog idel
    2    3  200    0    0    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    .2         18.
perm       phi        rhor       cr         rkml       rkmv       com        expan
20.   e-15 0.10       2550.      800.       2.         2.         0.          0.
tortx      diff0      texp       beta       bknud
0.50       2.6   e-05 1.   e-10 0.         0.0     e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
    7      0.45       9.6   e-04 1.0
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    7      0.45       1.0   e-03 8.   e-05 5.0  e+08 1.0
intmin     intmax
-11.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.   e-11 1.    e-2 1.    e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
123400.    0.0        232.6      0.0        -100.       0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.200e-13  phi0= 0.100e+00  rhor= 0.255e+04    cr= 0.800e+03
 rkml= 0.200e+01  rkmv= 0.200e+01   com= 0.        expan= 0.
tortx= 0.500e+00 diff0= 0.260e-04  texp= 0.100e-09
 beta= 0.        bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
  7  0.4500e+00 0.9600e-03 0.1000e+01 0.          0.          0.
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  7  0.4500e+00 0.1000e-02 0.8000e-04 0.5000e+09 0.1000e+01 0.

   Slr=0.9600e-03 Sltest=0.1264e-02   krl=0.8350e-18   krg=0.1000e+01
   pc2=-.1306e+13  denom=0.1090e-05

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           S0           Pa0
       0.100000e+06 0.200000e+00 0.979376e+05
       T0           Xga          Xla
       0.180000e+02 0.987057e+00 0.157570e-04

Integration Parameters
----------------------
etamin=0.1670e-04 etamax=0.6738e-02     zL=  -11.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.             Qe=0.              P=0.         T or S=0.
    Qa=0.             Pa=0.
 nzsav= 200        dzsav=0.3000e-01   ibat=0 ifxl=2 ifx2=3 ivpl= 0 idel= 1


 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1234e+06  0.2326e+03  -.1000e+03
 new  v=0.          0.          0.
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1234e+06  T= 232.6000
Sg=0.1000e+01 Pa=0.3720e-43 Xg=0.4823e-48 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3  , nok=270, nbad= 18
Qw=0.1860e-06 Qe=0.1410e-01 Qa=0.6154e-08  P=0.1038e+06  T=  16.6306
Sg=0.5245e-01 Pa=0.1019e+06 Xg=0.9886e+00 Xl=0.1639e-04

ith= 2
 old  v=0.1234e+06  0.2326e+03  -.1000e+03
 new  v=0.          0.          -.2000e+02
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1234e+06  T= 232.6000
Sg=0.1000e+01 Pa=0.2061e-08 Xg=0.2672e-13 Xl=0.
Ps too small, nstp=  127 iph=3 z=  -6.184
Try smaller Pa
 Qw=0.1593e-06  Qe=0.3504e+02   P=0.1135e+06 T/S=0.3449e+00
 Qa=0.1145e-07  Pa=0.1121e+06 S/T=0.1134e+02 Xga=0.9926e+00 Xla=0.1804e-04
```

Sample problem 2 output file.

```
ith= 3
 old  v=0.1234e+06  0.2326e+03  -.2000e+02
 new  v=0.          0.          -.5000e+02
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1234e+06  T= 232.6000
Sg=0.1000e+01 Pa=0.1929e-21 Xg=0.2500e-26 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3  , nok=217, nbad=  7
Qw=0.1646e-07 Qe=0.2468e-02 Qa=0.1008e-07  P=0.1082e+06  T=  12.6339
Sg=0.1795e+00 Pa=0.1068e+06 Xg=0.9916e+00 Xl=0.1718e-04

ith= 4
 old  v=0.1234e+06  0.2326e+03  -.5000e+02
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.7051e+01 seconds


 _________
|         |
|  Shoot  |
|_________|

-----------------------------------------------------------------------
Starting values for shot  1
   v=0.1234e+06  0.2326e+03  -.5000e+02
delv=0.1234e+04  0.2326e+01  -.5000e+00   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
2
 old
v=0.1234e+06 0.2326e+03 -.5000e+02  delv=0.1234e+04 0.2326e+01 -.5000e+00
 new
v=0.1134e+06 0.2380e+03 -.4500e+02  delv=0.         0.         0.
 new  eps=0.

Main    ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1134e+06  T= 238.0000
Sg=0.1000e+01 Pa=0.2863e-19 Xg=0.4041e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=201, nbad=  8
Qw=0.2012e-07 Qe=0.3240e-02 Qa=0.1074e-07  P=0.9799e+05  T=  16.7177
Sg=0.1902e+00 Pa=0.9609e+05 Xg=0.9878e+00 Xl=0.1546e-04

Delv(1) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1146e+06  T= 238.0000
Sg=0.1000e+01 Pa=0.2863e-19 Xg=0.3997e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=201, nbad=  8
Qw=0.1980e-07 Qe=0.3239e-02 Qa=0.1089e-07  P=0.9935e+05  T=  16.7655
Sg=0.1921e+00 Pa=0.9744e+05 Xg=0.9880e+00 Xl=0.1568e-04

Delv(2) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1134e+06  T= 240.3260
Sg=0.1000e+01 Pa=0.2863e-19 Xg=0.4041e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=191, nbad=  9
Qw=0.2233e-07 Qe=0.3749e-02 Qa=0.1127e-07  P=0.9800e+05  T=  18.9266
Sg=0.1919e+00 Pa=0.9581e+05 Xg=0.9860e+00 Xl=0.1541e-04

Delv(3) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1134e+06  T= 238.0000
Sg=0.1000e+01 Pa=0.1736e-19 Xg=0.2451e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=202, nbad=  8
Qw=0.2049e-07 Qe=0.3264e-02 Qa=0.1067e-07  P=0.9792e+05  T=  16.7900
Sg=0.1878e+00 Pa=0.9601e+05 Xg=0.9878e+00 Xl=0.1545e-04

Shot  1 results
vL=0.1134e+06  vU=0.9799e+05  dv/vcrit=0.1437e+01  f/fcrit=-.2006e+01
vL=0.2380e+03  vU=0.1902e+00  dv/vcrit=0.6185e+00  f/fcrit=-.4910e+01
vL=-.4500e+02  vU=0.1672e+02  dv/vcrit=-.2982e+01  f/fcrit=-.7124e+01
```

Sample problem 2 output file (continued).

```
-----------------------------------------------------------------------
Starting values for shot  2
   v=0.1151e+06  0.2395e+03  -.4370e+02
delv=0.1151e+04  0.2395e+01  -.4370e+00   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
0
Continue interactively (0) or switch to batch mode (1)
0

Main    ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 239.4811
Sg=0.1000e+01 Pa=0.1053e-18 Xg=0.1465e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=197, nbad=  7
Qw=0.2005e-07 Qe=0.3484e-02 Qa=0.1147e-07  P=0.9999e+05  T=  18.0030
Sg=0.2002e+00 Pa=0.9793e+05 Xg=0.9871e+00 Xl=0.1576e-04
All f < fcrit

Delv(1) ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1162e+06  T= 239.4811
Sg=0.1000e+01 Pa=0.1053e-18 Xg=0.1451e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=187, nbad=  7
Qw=0.1975e-07 Qe=0.3466e-02 Qa=0.1157e-07  P=0.1013e+06  T=  17.9615
Sg=0.2012e+00 Pa=0.9928e+05 Xg=0.9873e+00 Xl=0.1597e-04

Delv(2) ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 241.8759
Sg=0.1000e+01 Pa=0.1053e-18 Xg=0.1466e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=197, nbad= 10
Qw=0.2227e-07 Qe=0.4033e-02 Qa=0.1205e-07  P=0.9998e+05  T=  20.2906
Sg=0.2021e+00 Pa=0.9760e+05 Xg=0.9850e+00 Xl=0.1570e-04

Delv(3) ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 239.4811
Sg=0.1000e+01 Pa=0.6805e-19 Xg=0.9467e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=198, nbad=  7
Qw=0.2038e-07 Qe=0.3507e-02 Qa=0.1140e-07  P=0.9993e+05  T=  18.0690
Sg=0.1980e+00 Pa=0.9786e+05 Xg=0.9870e+00 Xl=0.1574e-04

Shot  2 results
vL=0.1151e+06  vU=0.9999e+05  dv/vcrit=0.8610e-02  f/fcrit=-.6312e-02
vL=0.2395e+03  vU=0.2002e+00  dv/vcrit=-.3455e-02  f/fcrit=0.8361e-01
vL=-.4370e+02  vU=0.1800e+02  dv/vcrit=0.7977e-01  f/fcrit=0.1662e-01

Converged, is= 2 CPU time=  24.324 seconds
```

Sample problem 2 output file (continued).

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
f-ode aa 1	-11.000000.		667.6700	1.23400	232.60000.		1	1	0
f-ode aa 1	-10.889820.	6227e-12	667.6595	1.23400	226.74620.	1448-108	4	1	1
f-ode aa 1	-10.664080.	2492e-11	667.6291	1.23400	214.75250.	5796-108	5	1	1
f-ode aa 1	-10.382260.	6630e-11	667.5657	1.23400	199.78060.	1542-107	6	1	1
f-ode aa 1	-10.078450.	1526e-10	667.4428	1.23400	183.64260.	3549-107	7	1	1
f-ode aa 1	-9.764650.	3316e-10	667.2073	1.23400	166.97830.	7714-107	8	1	1
f-ode aa 1	-9.447740.	7018e-10	666.7604	1.23400	150.15710.	1632-106	9	1	1
f-ode aa 1	-9.130860.	1466e-09	665.9190	1.23400	133.35290.	3409-106	10	1	1
f-ode aa 1	-8.815750.	3038e-09	664.3481	1.23400	116.67250.	7069-106	11	1	1
f-ode aa 1	-8.606360.	4936e-09	662.6049	1.23400	105.61600.	1149-105	0	1	0
f-ode aa 1	-8.606360.	4936e-09	662.6049	1.23400	105.61600.	1149-105	12	3	1
f-ode aa 1	-8.565680.	3814e-05	664.2157	1.22011	105.28830.	4784e-55	43	3	1
f-ode aa 1	-8.515630.	4885e-05	664.5865	1.20287	104.87700.	4548e-53	45	3	1
f-ode aa 1	-8.470180.	5658e-05	664.8214	1.18704	104.49520.	4255e-51	46	3	4
f-ode aa 1	-8.399710.	6805e-05	665.1334	1.16209	103.88490.	7089e-48	47	3	6
f-ode aa 1	-8.363440.	7426e-05	665.2908	1.14902	103.56080.	1041e-45	50	3	6
f-ode aa 1	-8.331570.	8008e-05	665.4338	1.13738	103.26950.	1322e-43	56	3	6
f-ode aa 1	-8.299780.	8633e-05	665.5842	1.12559	102.97190.	2784e-41	68	3	6
f-ode aa 1	-8.268210.	9307e-05	665.7436	1.11364	102.66790.	1086e-38	83	3	6
f-ode aa 1	-8.236990.	1003e-04	665.9127	1.10155	102.35730.	9236e-36	100	3	6
f-ode aa 1	-8.205740.	1083e-04	666.0935	1.08906	102.03370.	2548e-32	120	3	6
f-ode aa 1	-8.175020.	1169e-04	666.2807	1.07626	101.69870.	3378e-28	144	3	6
f-ode aa 1	-8.144310.	1261e-04	666.4706	1.06269	101.34000.	7015e-23	175	3	6
f-ode aa 1	-8.113800.	1359e-04	666.6460	1.04795	100.94580.	2441e-15	219	3	6
f-ode aa 1	-8.083430.	1409e-04	666.1895	1.04000	99.91570.	4925e-10	250	3	5
f-ode aa 1	-8.037830.	1419e-04	664.5966	1.03924	97.57190.	1879e-09	253	3	5
f-ode aa 1	-8.001310.	1425e-04	663.1870	1.03898	95.67580.	3023e-09	254	3	5
f-ode aa 1	-7.941680.	1434e-04	660.6433	1.03872	92.57780.	4943e-09	255	3	4
f-ode aa 1	-7.845970.	1450e-04	655.8724	1.03847	87.62030.	8163e-09	256	3	5
f-ode aa 1	-7.705490.	1475e-04	647.0444	1.03827	80.40610.	1322e-08	257	3	5
f-ode aa 1	-7.538590.	1512e-04	632.9597	1.03813	71.97280.	1979e-08	258	3	5
f-ode aa 1	-7.360570.	1560e-04	612.2458	1.03804	63.21210.	2756e-08	259	3	5
f-ode aa 1	-7.173810.	1619e-04	582.1297	1.03798	54.38660.	3679e-08	260	3	5
f-ode aa 1	-6.975030.	1692e-04	537.8036	1.03795	45.56770.	4827e-08	261	3	5
f-ode aa 1	-6.750150.	1776e-04	468.7551	1.03792	36.58420.	6444e-08	262	3	1
f-ode aa 1	-6.522980.	1839e-04	376.7349	1.03791	28.95470.	8623e-08	263	3	1
f-ode aa 1	-6.301320.	1839e-04	269.7305	1.03789	23.27200.	1156e-07	264	3	1
f-ode aa 1	-6.110270.	1753e-04	174.7547	1.03789	19.92440.	1494e-07	265	3	2
f-ode aa 1	-5.988330.	1643e-04	119.8680	1.03788	18.51430.	1755e-07	266	3	2
f-ode aa 1	-5.887470.	1518e-04	81.2769	1.03788	17.72170.	1994e-07	267	3	2
f-ode aa 1	-5.802210.	1389e-04	54.7915	1.03787	17.27080.	2209e-07	268	3	2
f-ode aa 1	-5.728190.	1262e-04	36.7365	1.03787	17.00920.	2403e-07	269	3	2
f-ode aa 1	-5.663100.	1141e-04	24.5820	1.03787	16.85630.	2577e-07	270	3	2
f-ode aa 1	-5.606040.	1030e-04	16.5616	1.03786	16.76720.	2729e-07	271	3	2
f-ode aa 1	-5.553990.	9266e-05	11.1253	1.03786	16.71330.	2866e-07	272	3	2
f-ode aa 1	-5.501920.	8227e-05	7.1968	1.03786	16.67840.	3000e-07	273	3	2
f-ode aa 1	-5.454970.	7304e-05	4.7050	1.03786	16.65850.	3118e-07	274	3	2
f-ode aa 1	-5.412200.	6484e-05	3.1147	1.03785	16.64700.	3220e-07	275	3	2
f-ode aa 1	-5.372870.	5758e-05	2.0934	1.03785	16.64030.	3310e-07	276	3	2
f-ode aa 1	-5.336470.	5116e-05	1.4333	1.03785	16.63630.	3389e-07	277	3	2
f-ode aa 1	-5.302480.	4547e-05	1.0021	1.03785	16.63400.	3459e-07	278	3	2
f-ode aa 1	-5.270180.	4037e-05	0.7151	1.03784	16.63260.	3521e-07	279	3	2
f-ode aa 1	-5.239440.	3582e-05	0.5232	1.03784	16.63180.	3576e-07	280	3	2
f-ode aa 1	-5.181710.	2815e-05	0.3040	1.03784	16.63100.	3669e-07	282	3	2
f-ode aa 1	-5.126670.	2193e-05	0.1947	1.03783	16.63070.	3744e-07	284	3	2
f-ode aa 1	-5.072070.	1684e-05	0.1342	1.03783	16.63060.	3805e-07	286	3	2
f-ode aa 1	-5.015950.	1268e-05	0.0966	1.03783	16.63060.	3855e-07	288	3	2
f-ode aa 1	-5.000000.	1169e-05	0.0886	1.03782	16.63060.	3867e-07	289	3	2

Sample problem 2 plot file (ith=1 preshot).

Label	z	$\ln(P_a)$ (bars)	S_g	Q_g (kg/s/m)	Q_l (kg/s/m)	X_g^a	NSTP	IPH	IERR
f-ode bb 1	-11.00000	-.1115e+030	.1000e+010	.	0.	0.4823e-48	1	1	0
f-ode bb 1	-10.88982	-.1115e+030	.1000e+010	.6227e-120	.	0.4823e-48	4	1	1
f-ode bb 1	-10.66408	-.1115e+030	.1000e+010	.2492e-110	.	0.4823e-48	5	1	1
f-ode bb 1	-10.38226	-.1115e+030	.1000e+010	.6630e-110	.	0.4823e-48	6	1	1
f-ode bb 1	-10.07845	-.1115e+030	.1000e+010	.1526e-100	.	0.4823e-48	7	1	1
f-ode bb 1	-9.76465	-.1115e+030	.1000e+010	.3316e-100	.	0.4823e-48	8	1	1
f-ode bb 1	-9.44774	-.1115e+030	.1000e+010	.7018e-100	.	0.4823e-48	9	1	1
f-ode bb 1	-9.13086	-.1115e+030	.1000e+010	.1466e-090	.	0.4823e-48	10	1	1
f-ode bb 1	-8.81575	-.1115e+030	.1000e+010	.3038e-090	.	0.4823e-48	11	1	1
f-ode bb 1	-8.60636	-.1115e+030	.1000e+010	.4936e-090	.	0.4823e-48	0	1	0
f-ode bb 1	-8.60636	-.1115e+030	.9987e+000	.2508e-03	-.2508e-03	0.4823e-48	12	3	1
f-ode bb 1	-8.56568	-.1084e+030	.6249e+000	.2499e-03	-.2461e-03	0.1031e-46	43	3	1
f-ode bb 1	-8.51563	-.1039e+030	.5310e+000	.2487e-03	-.2438e-03	0.9755e-45	45	3	1
f-ode bb 1	-8.47018	-.9935e+020	.4697e+000	.2475e-03	-.2418e-03	0.9468e-43	46	3	4
f-ode bb 1	-8.39971	-.9190e+020	.3888e+000	.2453e-03	-.2385e-03	0.1671e-39	47	3	6
f-ode bb 1	-8.36344	-.8688e+020	.3494e+000	.2440e-03	-.2366e-03	0.2552e-37	50	3	6
f-ode bb 1	-8.33157	-.8200e+020	.3151e+000	.2428e-03	-.2348e-03	0.3381e-35	56	3	6
f-ode bb 1	-8.29978	-.7661e+020	.2804e+000	.2413e-03	-.2326e-03	0.7524e-33	68	3	6
f-ode bb 1	-8.26821	-.7058e+020	.2454e+000	.2395e-03	-.2302e-03	0.3152e-30	83	3	6
f-ode bb 1	-8.23699	-.6376e+020	.2099e+000	.2374e-03	-.2273e-03	0.2937e-27	100	3	6
f-ode bb 1	-8.20574	-.5572e+020	.1734e+000	.2346e-03	-.2238e-03	0.9157e-24	120	3	6
f-ode bb 1	-8.17502	-.4608e+020	.1367e+000	.2309e-03	-.2192e-03	0.1429e-19	144	3	6
f-ode bb 1	-8.14431	-.3362e+020	.9928e-010	.2254e-03	-.2128e-03	0.3727e-14	175	3	6
f-ode bb 1	-8.11380	-.1593e+020	.6212e-010	.2162e-03	-.2026e-03	0.1815e-06	219	3	6
f-ode bb 1	-8.08343	-.3513e+010	.4445e-010	.1280e-04	0.1296e-05	0.4460e-01	250	3	5
f-ode bb 1	-8.03783	-.2201e+010	.4293e-010	.3266e-05	0.1092e-04	0.1589e+00	253	3	5
f-ode bb 1	-8.00131	-.1758e+010	.4245e-010	.1976e-05	0.1227e-04	0.2398e+00	254	3	5
f-ode bb 1	-7.94168	-.1324e+010	.4201e-010	.1163e-05	0.1318e-04	0.3534e+00	255	3	4
f-ode bb 1	-7.84597	-.9202e+000	.4167e-010	.6646e-06	0.1383e-04	0.4973e+00	256	3	5
f-ode bb 1	-7.70549	-.5855e+000	.4151e-010	.3768e-06	0.1438e-04	0.6481e+00	257	3	5
f-ode bb 1	-7.53859	-.3582e+000	.4157e-010	.2254e-06	0.1490e-04	0.7668e+00	258	3	5
f-ode bb 1	-7.36057	-.2141e+000	.4183e-010	.1420e-06	0.1546e-04	0.8483e+00	259	3	5
f-ode bb 1	-7.17381	-.1220e+000	.4225e-010	.9170e-07	0.1611e-04	0.9026e+00	260	3	5
f-ode bb 1	-6.97503	-.6263e-010	.4286e-010	.5960e-07	0.1687e-04	0.9385e+00	261	3	5
f-ode bb 1	-6.75015	-.2369e-010	.4379e-010	.3837e-07	0.1773e-04	0.9623e+00	262	3	1
f-ode bb 1	-6.52298	-.2032e-020	.4499e-010	.2677e-07	0.1837e-04	0.9757e+00	263	3	1
f-ode bb 1	-6.30132	0.9309e-020	.4641e-010	.2157e-07	0.1838e-04	0.9827e+00	264	3	1
f-ode bb 1	-6.11027	0.1452e-010	.4778e-010	.2053e-07	0.1752e-04	0.9859e+00	265	3	2
f-ode bb 1	-5.98833	0.1645e-010	.4867e-010	.2117e-07	0.1643e-04	0.9871e+00	266	3	2
f-ode bb 1	-5.88747	0.1746e-010	.4938e-010	.2234e-07	0.1518e-04	0.9878e+00	267	3	2
f-ode bb 1	-5.80221	0.1801e-010	.4994e-010	.2373e-07	0.1389e-04	0.9881e+00	268	3	2
f-ode bb 1	-5.72819	0.1833e-010	.5040e-010	.2517e-07	0.1262e-04	0.9883e+00	269	3	2
f-ode bb 1	-5.66310	0.1851e-010	.5077e-010	.2658e-07	0.1141e-04	0.9884e+00	270	3	2
f-ode bb 1	-5.60604	0.1861e-010	.5106e-010	.2790e-07	0.1030e-04	0.9885e+00	271	3	2
f-ode bb 1	-5.55399	0.1867e-010	.5130e-010	.2915e-07	0.9265e-05	0.9885e+00	272	3	2
f-ode bb 1	-5.50192	0.1871e-010	.5151e-010	.3041e-07	0.8227e-05	0.9885e+00	273	3	2
f-ode bb 1	-5.45497	0.1873e-010	.5169e-010	.3154e-07	0.7303e-05	0.9886e+00	274	3	2
f-ode bb 1	-5.41220	0.1874e-010	.5182e-010	.3254e-07	0.6484e-05	0.9886e+00	275	3	2
f-ode bb 1	-5.37287	0.1875e-010	.5194e-010	.3344e-07	0.5758e-05	0.9886e+00	276	3	2
f-ode bb 1	-5.33647	0.1875e-010	.5203e-010	.3423e-07	0.5115e-05	0.9886e+00	277	3	2
f-ode bb 1	-5.30248	0.1875e-010	.5211e-010	.3493e-07	0.4546e-05	0.9886e+00	278	3	2
f-ode bb 1	-5.27018	0.1875e-010	.5217e-010	.3556e-07	0.4037e-05	0.9886e+00	279	3	2
f-ode bb 1	-5.23944	0.1875e-010	.5222e-010	.3612e-07	0.3582e-05	0.9886e+00	280	3	2
f-ode bb 1	-5.18171	0.1875e-010	.5231e-010	.3707e-07	0.2814e-05	0.9886e+00	282	3	2
f-ode bb 1	-5.12667	0.1874e-010	.5236e-010	.3784e-07	0.2193e-05	0.9886e+00	284	3	2
f-ode bb 1	-5.07207	0.1874e-010	.5241e-010	.3846e-07	0.1683e-05	0.9886e+00	286	3	2
f-ode bb 1	-5.01595	0.1874e-010	.5244e-010	.3897e-07	0.1268e-05	0.9886e+00	288	3	2
f-ode bb 1	-5.00000	0.1874e-010	.5245e-010	.3904e-07	0.1217e-05	0.9886e+00	289	3	2

Sample problem 2 plot file (ith=1 preshot).

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
p-ode aa 2	-11.000000.		667.6700	1.23400	232.60000.		1	1	2
p-ode aa 2	-10.904550.	5303e-12	667.6610	1.23400	227.52880.	3787e-39	4	1	1
p-ode aa 2	-10.697820.	2149e-11	667.6345	1.23400	216.54510.	1535e-38	5	1	1
p-ode aa 2	-10.420830.	5898e-11	667.5766	1.23400	201.82980.	4211e-38	6	1	1
p-ode aa 2	-10.118940.	1374e-10	667.4638	1.23400	185.79310.	9811e-38	7	1	1
p-ode aa 2	-9.805760.	3004e-10	667.2472	1.23400	169.16090.	2145e-37	8	1	1
p-ode aa 2	-9.489430.	6366e-10	666.8365	1.23400	152.36920.	4546e-37	9	1	1
p-ode aa 2	-9.172360.	1331e-09	666.0617	1.23400	135.55250.	9507e-37	10	1	1
p-ode aa 2	-8.856920.	2762e-09	664.6134	1.23400	118.84930.	1973e-36	11	1	1
p-ode aa 2	-8.606360.	4936e-09	662.6049	1.23400	105.61600.	3526e-36	0	1	0
p-ode aa 2	-8.606360.	4936e-09	662.6049	1.23400	105.61600.	3526e-36	12	3	1
p-ode aa 2	-8.572180.	3629e-05	664.1458	1.22234	105.34110.	1488e-20	44	3	5
p-ode aa 2	-8.539750.	4421e-05	664.4325	1.21120	105.07640.	2658e-19	51	3	5
p-ode aa 2	-8.506170.	5053e-05	664.6398	1.19959	104.79830.	6554e-18	59	3	6
p-ode aa 2	-8.475420.	5572e-05	664.7966	1.18887	104.53960.	1609e-16	67	3	6
p-ode aa 2	-8.443480.	6090e-05	664.9432	1.17765	104.26670.	5890e-15	76	3	6
p-ode aa 2	-8.410790.	6622e-05	665.0856	1.16605	103.98230.	3207e-13	86	3	6
p-ode aa 2	-8.380560.	7126e-05	665.2128	1.15527	103.70850.	1733e-11	96	3	6
p-ode aa 2	-8.346100.	7608e-05	665.1945	1.14539	103.08170.	8675e-10	106	3	6
p-ode aa 2	-8.305190.	7819e-05	664.6251	1.14149	101.38780.	4425e-09	110	3	5
p-ode aa 2	-8.249180.	7948e-05	663.5138	1.13951	98.67110.	1050e-08	112	3	5
p-ode aa 2	-8.197640.	8029e-05	662.3078	1.13851	96.07870.	1655e-08	113	3	5
p-ode aa 2	-8.117160.	8130e-05	660.1067	1.13752	91.97430.	2661e-08	114	3	5
p-ode aa 2	-7.994610.	8260e-05	655.9415	1.13662	85.68680.	4323e-08	115	3	5
p-ode aa 2	-7.833150.	8415e-05	648.6176	1.13592	77.41870.	6761e-08	116	3	5
p-ode aa 2	-7.656180.	8564e-05	637.4259	1.13548	68.44790.	9798e-08	117	3	5
p-ode aa 2	-7.471840.	8674e-05	620.9672	1.13520	59.27960.	1346e-07	118	3	5
p-ode aa 2	-7.278870.	8673e-05	596.5636	1.13503	49.97470.	1803e-07	119	3	1
p-ode aa 2	-7.104140.	8458e-05	566.0529	1.13493	41.91820.	2308e-07	120	3	1
p-ode aa 2	-6.944270.	7951e-05	529.2854	1.13486	34.96630.	2876e-07	121	3	1
p-ode aa 2	-6.797880.	7105e-05	486.8686	1.13482	29.05620.	3511e-07	122	3	1
p-ode aa 2	-6.649720.	5812e-05	434.6149	1.13479	23.62700.	4284e-07	123	3	1
p-ode aa 2	-6.515890.	4331e-05	379.4137	1.13477	19.29350.	5087e-07	124	3	1
p-ode aa 2	-6.392610.	2894e-05	322.7709	1.13476	15.84930.	5881e-07	125	3	1
p-ode aa 2	-6.307440.	1997e-05	281.3499	1.13475	13.80320.	6432e-07	126	3	1
p-ode aa 2	-6.241320.	1411e-05	248.5528	1.13474	12.41010.	6847e-07	127	3	1

Sample problem 2 plot file (ith=2 preshot).

Label	z	$\ln(P_a)$ (bars)	S_g	Q_g (kg/s/m)	Q_l (kg/s/m)	X_g^a	NSTP	IPH	IERR
p-ode bb 2	-11.00000	-.3151e+020	.1000e+010	.	0.	0.2672e-13	1	1	2
p-ode bb 2	-10.90455	-.3151e+020	.1000e+010	.5303e-12	0.	0.2672e-13	4	1	1
p-ode bb 2	-10.69782	-.3151e+020	.1000e+010	.2149e-11	0.	0.2672e-13	5	1	1
p-ode bb 2	-10.42083	-.3151e+020	.1000e+010	.5898e-11	0.	0.2672e-13	6	1	1
p-ode bb 2	-10.11894	-.3151e+020	.1000e+010	.1374e-10	0.	0.2672e-13	7	1	1
p-ode bb 2	-9.80576	-.3151e+020	.1000e+010	.3004e-10	0.	0.2672e-13	8	1	1
p-ode bb 2	-9.48943	-.3151e+020	.1000e+010	.6366e-10	0.	0.2672e-13	9	1	1
p-ode bb 2	-9.17236	-.3151e+020	.1000e+010	.1331e-09	0.	0.2672e-13	10	1	1
p-ode bb 2	-8.85692	-.3150e+020	.1000e+010	.2762e-09	0.	0.2672e-13	11	1	1
p-ode bb 2	-8.60636	-.3150e+020	.1000e+010	.4936e-09	0.	0.2672e-13	0	1	0
p-ode bb 2	-8.60636	-.3150e+020	.9987e+000	.2508e-03	-.2508e-03	0.2672e-13	12	3	1
p-ode bb 2	-8.57218	-.2899e+020	.6421e+000	.2500e-03	-.2464e-03	0.3333e-12	44	3	5
p-ode bb 2	-8.53975	-.2618e+020	.5705e+000	.2493e-03	-.2448e-03	0.5592e-11	51	3	5
p-ode bb 2	-8.50617	-.2295e+020	.5172e+000	.2484e-03	-.2434e-03	0.1417e-09	59	3	6
p-ode bb 2	-8.47542	-.1974e+020	.4762e+000	.2476e-03	-.2420e-03	0.3567e-08	67	3	6
p-ode bb 2	-8.44348	-.1612e+020	.4378e+000	.2467e-03	-.2406e-03	0.1338e-06	76	3	6
p-ode bb 2	-8.41079	-.1211e+020	.4009e+000	.2456e-03	-.2390e-03	0.7485e-05	86	3	6
p-ode bb 2	-8.38056	-.8097e+010	.3681e+000	.2399e-03	-.2328e-03	0.4164e-03	96	3	6
p-ode bb 2	-8.34610	-.4169e+010	.3388e+000	.1152e-03	-.1076e-03	0.2118e-01	106	3	6
p-ode bb 2	-8.30519	-.2564e+010	.3276e+000	.3473e-04	-.2691e-04	0.1027e+00	110	3	5
p-ode bb 2	-8.24918	-.1752e+010	.3222e+000	.1539e-04	-.7441e-05	0.2213e+00	112	3	5
p-ode bb 2	-8.19764	-.1350e+010	.3198e+000	.9739e-05	-.1708e-05	0.3183e+00	113	3	5
p-ode bb 2	-8.11716	-.9619e+000	.3177e+000	.5922e-05	0.2211e-05	0.4453e+00	114	3	5
p-ode bb 2	-7.99461	-.6109e+000	.3164e+000	.3470e-05	0.4795e-05	0.5924e+00	115	3	5
p-ode bb 2	-7.83315	-.3429e+000	.3162e+000	.2047e-05	0.6375e-05	0.7263e+00	116	3	5
p-ode bb 2	-7.65618	-.1694e+000	.3173e+000	.1271e-05	0.7303e-05	0.8223e+00	117	3	5
p-ode bb 2	-7.47184	-.5917e-01	0.3194e+000	.8147e-06	0.7873e-05	0.8867e+00	118	3	5
p-ode bb 2	-7.27887	0.1176e-01	0.3225e+000	.5263e-06	0.8164e-05	0.9294e+00	119	3	1
p-ode bb 2	-7.10414	0.5192e-01	0.3260e+000	.3603e-06	0.8121e-05	0.9539e+00	120	3	1
p-ode bb 2	-6.94427	0.7581e-01	0.3298e+000	.2591e-06	0.7721e-05	0.9686e+00	121	3	1
p-ode bb 2	-6.79788	0.9044e-01	0.3335e+000	.1963e-06	0.6944e-05	0.9776e+00	122	3	1
p-ode bb 2	-6.64972	0.1004e+000	.3374e+000	.1540e-06	0.5701e-05	0.9838e+00	123	3	1
p-ode bb 2	-6.51589	0.1065e+000	.3405e+000	.1293e-06	0.4252e-05	0.9876e+00	124	3	1
p-ode bb 2	-6.39261	0.1104e+000	.3427e+000	.1149e-06	0.2838e-05	0.9901e+00	125	3	1
p-ode bb 2	-6.30744	0.1124e+000	.3438e+000	.1084e-06	0.1953e-05	0.9913e+00	126	3	1
p-ode bb 2	-6.24132	0.1136e+000	.3445e+000	.1047e-06	0.1375e-05	0.9921e+00	127	3	1

Sample problem 2 plot file (ith=2 preshot).

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
aa	20	-11.000000.	667.6700	1.15053	239.48110.		1	1	2
aa	20	-10.969810.1409e-12	667.6673	1.15053	237.87720.3026e-60		3	1	1
aa	20	-10.881570.6112e-12	667.6586	1.15053	233.18860.1313e-59		4	1	1
aa	20	-10.647540.2413e-11	667.6263	1.15053	220.75490.5182e-59		5	1	1
aa	20	-10.363150.6335e-11	667.5600	1.15053	205.64650.1361e-58		6	1	1
aa	20	-10.057690.1451e-10	667.4314	1.15053	189.42110.3116e-58		7	1	1
aa	20	-9.742470.3148e-10	667.1844	1.15053	172.68190.6762e-58		8	1	1
aa	20	-9.424100.6660e-10	666.7143	1.15053	155.78400.1431e-57		9	1	1
aa	20	-9.105630.1392e-09	665.8263	1.15053	138.89740.2989e-57		10	1	1
aa	20	-8.788560.2888e-09	664.1605	1.15053	122.11620.6205e-57		11	1	1
aa	20	-8.474060.5966e-09	661.0654	1.15053	105.52900.1282e-56		12	1	1
aa	20	-8.437350.6495e-09	660.5616	1.15053	103.59840.1396e-56		0	1	0
aa	20	-8.437350.6495e-09	660.5616	1.15053	103.59840.1396e-56		13	3	1
aa	20	-8.403810.5057e-05	662.6600	1.13868	103.30210.9312e-31		41	3	6
aa	20	-8.370040.6216e-05	663.0605	1.12666	102.99910.1732e-29		48	3	6
aa	20	-8.339620.7025e-05	663.3104	1.11575	102.72180.2867e-28		55	3	6
aa	20	-8.307680.7788e-05	663.5256	1.10421	102.42600.7043e-27		63	3	6
aa	20	-8.274600.8547e-05	663.7233	1.09216	102.11430.2578e-25		72	3	6
aa	20	-8.244070.9252e-05	663.8954	1.08093	101.82130.9412e-24		81	3	6
aa	20	-8.212800.9997e-05	664.0691	1.06931	101.51540.5104e-22		91	3	6
aa	20	-8.181290.1079e-04	664.2473	1.05746	101.20060.4103e-20		102	3	6
aa	20	-8.150080.1163e-04	664.4312	1.04556	100.88150.4882e-18		114	3	6
aa	20	-8.119700.1252e-04	664.6210	1.03377	100.56260.8581e-16		127	3	6
aa	20	-8.088700.1350e-04	664.8278	1.02150	100.22710.3307e-13		142	3	6
aa	20	-8.058640.1449e-04	664.9770	1.00992	99.82640.1784e-10		158	3	6
aa	20	-8.023350.1493e-04	664.1745	1.00525	98.43520.2840e-09		165	3	5
aa	20	-7.985790.1509e-04	662.8453	1.00389	96.59990.6632e-09		167	3	5
aa	20	-7.951240.1519e-04	661.4648	1.00320	94.86090.1032e-08		168	3	5
aa	20	-7.897100.1532e-04	659.0530	1.00251	92.10570.1633e-08		169	3	5
aa	20	-7.811680.1549e-04	654.6288	1.00184	87.74070.2633e-08		170	3	5
aa	20	-7.682860.1573e-04	646.3416	1.00124	81.18220.4255e-08		171	3	5
aa	20	-7.518780.1604e-04	632.3062	1.00080	72.93750.6541e-08		172	3	5
aa	20	-7.339530.1637e-04	611.1589	1.00051	64.15440.9366e-08		173	3	5
aa	20	-7.149680.1667e-04	579.9853	1.00034	55.22380.1284e-07		174	3	5
aa	20	-6.944420.1682e-04	533.0601	1.00022	46.18310.1736e-07		175	3	1
aa	20	-6.727110.1648e-04	464.9325	1.00015	37.58300.2343e-07		176	3	1
aa	20	-6.530540.1532e-04	385.5851	1.00011	30.94990.3054e-07		177	3	1
aa	20	-6.345490.1313e-04	297.8783	1.00008	25.93330.3890e-07		178	3	1
aa	20	-6.173300.1009e-04	211.3492	1.00006	22.46200.4786e-07		179	3	1
aa	20	-6.018150.6907e-05	137.6686	1.00004	20.32660.5606e-07		180	3	1
aa	20	-5.907700.4742e-05	92.5390	1.00003	19.32530.6129e-07		181	3	2
aa	20	-5.816880.3217e-05	62.0846	1.00002	18.77310.6489e-07		182	3	2
aa	20	-5.739650.2175e-05	41.5598	1.00001	18.45860.6732e-07		183	3	2
aa	20	-5.673930.1489e-05	28.0315	1.00000	18.27900.6892e-07		184	3	1
aa	20	-5.615910.1032e-05	18.9155	1.00000	18.17210.6999e-07		185	3	1
aa	20	-5.563590.7256e-06	12.7326	0.99999	18.10720.7071e-07		186	3	1
aa	20	-5.510860.5039e-06	8.1771	0.99999	18.06410.7123e-07		187	3	1
aa	20	-5.463060.3640e-06	5.2487	0.99998	18.03910.7157e-07		188	3	1
aa	20	-5.419220.2756e-06	3.3637	0.99998	18.02440.7177e-07		189	3	2
aa	20	-5.378770.2200e-06	2.1545	0.99997	18.01570.7190e-07		190	3	2
aa	20	-5.341560.1853e-06	1.3860	0.99997	18.01060.7198e-07		191	3	2
aa	20	-5.307330.1636e-06	0.8988	0.99997	18.00760.7203e-07		192	3	2
aa	20	-5.275120.1498e-06	0.5838	0.99996	18.00580.7206e-07		193	3	2
aa	20	-5.216970.1357e-06	0.2541	0.99996	18.00400.7208e-07		195	3	2
aa	20	-5.164940.1299e-06	0.1169	0.99995	18.00340.7209e-07		197	3	2
aa	20	-5.117370.1275e-06	0.0594	0.99995	18.00310.7208e-07		199	3	2
aa	20	-5.073230.1265e-06	0.0353	0.99994	18.00300.7207e-07		201	3	2
aa	20	-5.030490.1261e-06	0.0252	0.99994	18.00300.7206e-07		203	3	2
aa	20	-5.000000.1260e-06	0.0219	0.99994	18.00300.7205e-07		205	3	2

Sample problem 2 plot file (is=2 shot).

Label	z	$\ln(P_a)$ (bars)	S_g	Q_g (kg/s/m)	$\dot{Q}_l$ (kg/s/m)	X_g^a	NSTP	IPH	IERR
bb 20	-11.00000	-.5521e+020	.1000e+010	.	0.	0.1465e-23	1	1	2
bb 20	-10.96981	-.5521e+020	.1000e+010	.1409e-120	.	0.1465e-23	3	1	1
bb 20	-10.88157	-.5521e+020	.1000e+010	.6112e-120	.	0.1465e-23	4	1	1
bb 20	-10.64754	-.5521e+020	.1000e+010	.2413e-110	.	0.1465e-23	5	1	1
bb 20	-10.36315	-.5521e+020	.1000e+010	.6335e-110	.	0.1465e-23	6	1	1
bb 20	-10.05769	-.5521e+020	.1000e+010	.1451e-100	.	0.1465e-23	7	1	1
bb 20	-9.74247	-.5521e+020	.1000e+010	.3148e-100	.	0.1465e-23	8	1	1
bb 20	-9.42410	-.5521e+020	.1000e+010	.6660e-100	.	0.1465e-23	9	1	1
bb 20	-9.10563	-.5520e+020	.1000e+010	.1392e-090	.	0.1466e-23	10	1	1
bb 20	-8.78856	-.5520e+020	.1000e+010	.2888e-090	.	0.1466e-23	11	1	1
bb 20	-8.47406	-.5520e+020	.1000e+010	.5966e-090	.	0.1466e-23	12	1	1
bb 20	-8.43735	-.5520e+020	.1000e+010	.6495e-090	.	0.1466e-23	0	1	0
bb 20	-8.43735	-.5520e+020	.9987e+000	.2449e-03	-.2449e-03	0.1466e-23	13	3	1
bb 20	-8.40381	-.5281e+020	.6447e+000	.2440e-03	-.2390e-03	0.1615e-22	41	3	6
bb 20	-8.37004	-.4997e+020	.5702e+000	.2431e-03	-.2369e-03	0.2784e-21	48	3	6
bb 20	-8.33962	-.4715e+020	.5215e+000	.2422e-03	-.2352e-03	0.4722e-20	55	3	6
bb 20	-8.30768	-.4393e+020	.4785e+000	.2412e-03	-.2334e-03	0.1192e-18	63	3	6
bb 20	-8.27460	-.4032e+020	.4384e+000	.2401e-03	-.2316e-03	0.4480e-17	72	3	6
bb 20	-8.24407	-.3670e+020	.4035e+000	.2390e-03	-.2297e-03	0.1680e-15	81	3	6
bb 20	-8.21280	-.3269e+020	.3688e+000	.2378e-03	-.2278e-03	0.9412e-14	91	3	6
bb 20	-8.18129	-.2827e+020	.3342e+000	.2364e-03	-.2256e-03	0.7877e-12	102	3	6
bb 20	-8.15008	-.2345e+020	.2997e+000	.2348e-03	-.2232e-03	0.9855e-10	114	3	6
bb 20	-8.11970	-.1823e+020	.2656e+000	.2330e-03	-.2205e-03	0.1844e-07	127	3	6
bb 20	-8.08870	-.1221e+020	.2299e+000	.2307e-03	-.2172e-03	0.7721e-05	142	3	6
bb 20	-8.05864	-.5833e+010	.1962e+000	.1661e-03	-.1516e-03	0.4582e-02	158	3	6
bb 20	-8.02335	-.3051e+010	.1829e+000	.2942e-04	-.1449e-04	0.7253e-01	165	3	5
bb 20	-7.98579	-.2229e+010	.1792e+000	.1303e-04	0.2064e-05	0.1598e+00	167	3	5
bb 20	-7.95124	-.1819e+010	.1775e+000	.8317e-05	0.6877e-05	0.2342e+00	168	3	5
bb 20	-7.89710	-.1413e+010	.1759e+000	.5140e-05	0.1018e-04	0.3373e+00	169	3	5
bb 20	-7.81168	-.1025e+010	.1746e+000	.3061e-05	0.1243e-04	0.4700e+00	170	3	5
bb 20	-7.68286	-.6842e+000	.1740e+000	.1770e-05	0.1397e-04	0.6179e+00	171	3	5
bb 20	-7.51878	-.4348e+000	.1742e+000	.1045e-05	0.1500e-04	0.7450e+00	172	3	5
bb 20	-7.33953	-.2748e+000	.1754e+000	.6483e-06	0.1573e-04	0.8345e+00	173	3	5
bb 20	-7.14968	-.1729e+000	.1773e+000	.4124e-06	0.1628e-04	0.8943e+00	174	3	5
bb 20	-6.94442	-.1071e+000	.1800e+000	.2624e-06	0.1658e-04	0.9340e+00	175	3	1
bb 20	-6.72711	-.6679e-01	0.1838e+000	.1693e-06	0.1634e-04	0.9586e+00	176	3	1
bb 20	-6.53054	-.4571e-01	0.1877e+000	.1205e-06	0.1523e-04	0.9716e+00	177	3	1
bb 20	-6.34549	-.3396e-01	0.1916e+000	.9443e-07	0.1307e-04	0.9789e+00	178	3	1
bb 20	-6.17330	-.2749e-01	0.1949e+000	.8175e-07	0.1006e-04	0.9829e+00	179	3	1
bb 20	-6.01815	-.2409e-01	0.1973e+000	.7641e-07	0.6887e-05	0.9850e+00	180	3	1
bb 20	-5.90770	-.2263e-01	0.1985e+000	.7468e-07	0.4728e-05	0.9859e+00	181	3	2
bb 20	-5.81688	-.2187e-01	0.1992e+000	.7396e-07	0.3208e-05	0.9864e+00	182	3	2
bb 20	-5.73965	-.2144e-01	0.1996e+000	.7362e-07	0.2169e-05	0.9867e+00	183	3	2
bb 20	-5.67393	-.2121e-01	0.1998e+000	.7345e-07	0.1485e-05	0.9868e+00	184	3	1
bb 20	-5.61591	-.2107e-01	0.2000e+000	.7334e-07	0.1028e-05	0.9869e+00	185	3	1
bb 20	-5.56359	-.2099e-01	0.2000e+000	.7327e-07	0.7231e-06	0.9870e+00	186	3	1
bb 20	-5.51086	-.2094e-01	0.2001e+000	.7321e-07	0.5019e-06	0.9870e+00	187	3	1
bb 20	-5.46306	-.2091e-01	0.2001e+000	.7317e-07	0.3624e-06	0.9870e+00	188	3	1
bb 20	-5.41922	-.2089e-01	0.2001e+000	.7314e-07	0.2743e-06	0.9870e+00	189	3	2
bb 20	-5.37877	-.2089e-01	0.2002e+000	.7312e-07	0.2188e-06	0.9870e+00	190	3	2
bb 20	-5.34156	-.2088e-01	0.2002e+000	.7310e-07	0.1842e-06	0.9870e+00	191	3	2
bb 20	-5.30733	-.2088e-01	0.2002e+000	.7308e-07	0.1626e-06	0.9871e+00	192	3	2
bb 20	-5.27512	-.2088e-01	0.2002e+000	.7307e-07	0.1488e-06	0.9871e+00	193	3	2
bb 20	-5.21697	-.2089e-01	0.2002e+000	.7305e-07	0.1347e-06	0.9871e+00	195	3	2
bb 20	-5.16494	-.2089e-01	0.2002e+000	.7304e-07	0.1290e-06	0.9871e+00	197	3	2
bb 20	-5.11737	-.2090e-01	0.2002e+000	.7303e-07	0.1266e-06	0.9871e+00	199	3	2
bb 20	-5.07323	-.2090e-01	0.2002e+000	.7301e-07	0.1256e-06	0.9871e+00	201	3	2
bb 20	-5.03049	-.2090e-01	0.2002e+000	.7300e-07	0.1252e-06	0.9871e+00	203	3	2
bb 20	-5.00000	-.2091e-01	0.2002e+000	.7299e-07	0.1251e-06	0.9871e+00	205	3	2

Sample problem 2 plot file (is=2 shot).

Problem 3: Low permeability medium, vapor pressure lowering (input and output files shown)

With vapor pressure lowering included (IVPL=1) it is not known *a priori* what the phase conditions will be at ZL. Single-phase conditions are specified for V at ZL (see input file), and SIMSOL converts them to two-phase conditions if vapor pressure lowering is strong enough (see output file).

Sample problem 3 input file.

```
 ifxl ifx2   nz ibat ivpl ilog idel
    0    3  200    0    1    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    .3         22.
perm       phi        rhor       cr         rkml       rkmv       com        expan
1.9   e-18 0.1        2480.      840.       2.34       1.90       0.          0.
tortx      diff0      texp       beta       bknud
0.25       2.14  e-05 2.334e-00 0.          0.0     e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
    7      0.4438     0.0801      1.        .0018      1.    e-11 1.
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    7      0.4438     8.01  e-02 5.792e-07 5.0  e+08 1.0       1.0    e-04
intmin     intmax
-12.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.   e-11 1.    e-2 1.    e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
1237500.   0.0        291.08     0.0        .1957 e+06 0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.190e-17  phi0= 0.100e+00  rhor= 0.248e+04    cr= 0.840e+03
 rkml= 0.234e+01  rkmv= 0.190e+01   com= 0.        expan= 0.
tortx= 0.250e+00 diff0= 0.214e-04  texp= 0.233e+01
 beta= 0.        bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
  7  0.4438e+00 0.8010e-01 0.1000e+01 0.1800e-02 0.1000e-10 0.1000e+01
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  7  0.4438e+00 0.8010e-01 0.5792e-06 0.5000e+09 0.1000e+01 0.1000e-03

   Slr=0.8010e-01 Sltest=0.8057e-01   krl=0.6713e-17   krg=0.1000e+01
   pc2=-.2070e+12  denom=0.1389e-05

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           S0           Pa0
       0.100000e+06 0.300000e+00 0.973985e+05
       T0           Xga          Xla
       0.220000e+02 0.983637e+00 0.156702e-04

Integration Parameters
----------------------
etamin=0.6144e-05 etamax=0.6738e-02     zL=  -12.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.             Qe=0.              P=0.         T or S=0.
    Qa=0.             Pa=0.
 nzsav= 200        dzsav=0.3500e-01   ibat=0 ifxl=0 ifx2=3 ivpl= 1 idel= 1

 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1237e+07  0.2911e+03  0.1957e+06
 new  v=0.          0.          0.
 old   zL= -12.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -12.000, iph=3
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1237e+07  T= 291.0800
Sg=0.9072e+00 Pa=0.1957e+06 Xg=0.2270e+00 Xl=0.3149e-04
        ODEINT done,    zU=  -5.000, iph=3  , nok=371, nbad=133
Qw=0.2820e-12 Qe=0.2083e-02 Qa=-.2234e-12  P=0.1000e+06  T=  22.0039
Sg=0.3001e+00 Pa=0.9740e+05 Xg=0.9836e+00 Xl=0.1567e-04
Converged

ith= 2
 old  v=0.1237e+07  0.2911e+03  0.1957e+06
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.1130e+02 seconds

 _________
|         |
|  Shoot  |
|_________|

-----------------------------------------------------------------------
Starting values for shot  1
   v=0.1237e+07  0.2911e+03  0.1957e+06
delv=0.1237e+05  0.2911e+01  0.1957e+04   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
1
Stop
```

Sample problem 3 output file.

Problem 4: Effective continuum, sequential-saturation model (input and output files shown)

For the sequential-saturation model of a fractured/porous medium, the characteristic curves IRP=11 and ICP=8 are used (see input file).

Sample problem 4 input file.

```
 ifx1 ifx2   nz ibat ivpl ilog idel
    2    3  200    0    1    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    .3         22.
perm       phi        rhor       cr         rkml       rkmv       com        expan
1.9   e-18 0.1        2480.      840.       2.34       1.90       0.          0.
tortx      diff0      texp       beta       bknud
0.25       2.14  e-05 2.334e-00 0.          0.0     e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
   11      0.4438     0.0801      1.        .0018      1.    e-11 1.
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    8      0.4438     0.0801      5.792e-07 5.0  e+08 1.0       1.0   e-04
intmin     intmax
-11.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.   e-11 1.    e-2 1.    e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
103000.    0.0        245.54     0.0        -31.8      0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.190e-17  phi0= 0.100e+00  rhor= 0.248e+04    cr= 0.840e+03
 rkml= 0.234e+01  rkmv= 0.190e+01   com= 0.        expan= 0.
tortx= 0.250e+00 diff0= 0.214e-04  texp= 0.233e+01
 beta= 0.        bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
 11  0.4438e+00 0.8010e-01 0.1000e+01 0.1800e-02 0.1000e-10 0.1000e+01
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  8  0.4438e+00 0.8010e-01 0.5792e-06 0.5000e+09 0.1000e+01 0.1000e-03

   Slr=0.7868e-01 Sltest=0.8183e-01   krl=0.1022e-16   krg=0.1000e+01
   pc2=-.1497e+12  denom=0.1530e-05

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           S0           Pa0
       0.100000e+06 0.300000e+00 0.973968e+05
       T0           Xga          Xla
       0.220000e+02 0.983627e+00 0.156700e-04

Integration Parameters
----------------------
etamin=0.1670e-04 etamax=0.6738e-02     zL=  -11.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.              Qe=0.              P=0.         T or S=0.
    Qa=0.              Pa=0.
 nzsav= 200        dzsav=0.3000e-01   ibat=0 ifx1=2 ifx2=3 ivpl= 1 idel= 1

 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1030e+06  0.2455e+03  -.3180e+02
 new  v=0.          0.          0.
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=3
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1030e+06  T= 245.5400
Sg=0.9140e+00 Pa=0.1547e-13 Xg=0.2405e-18 Xl=0.2489e-23
        ODEINT done,     zU=  -5.000, iph=3  , nok=446, nbad=108
Qw=0.2295e-09 Qe=0.4042e-02 Qa=0.1374e-07  P=0.9998e+05  T=  21.9903
Sg=0.2981e+00 Pa=0.9738e+05 Xg=0.9836e+00 Xl=0.1567e-04
Converged

ith= 2
 old  v=0.1030e+06  0.2455e+03  -.3180e+02
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.1180e+02 seconds

 _________
|         |
|  Shoot  |
|_________|

-----------------------------------------------------------------------
Starting values for shot  1
   v=0.1030e+06  0.2455e+03  -.3180e+02
delv=0.1030e+04  0.2455e+01  -.3180e+00   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
1
Stop
```

Sample problem 4 output file.

Problem 5: Effective continuum, curve-fit to concurrent-saturation model (input and output files shown)

For the curve-fit concurrent-saturation model of a fractured/porous medium, the characteristic curves IRP=12 and ICP=8 are used (see input file). Figure 2 shows how the curve-fit parameters control the shape of the liquid relative permeability curve.

Sample problem 5 input file.

```
 ifx1 ifx2   nz ibat ivpl ilog idel
    2    3  200    0    1    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    .3         22.
perm       phi        rhor       cr         rkml       rkmv       com        expan
1.9   e-18 0.10       2480.      840.       2.34       1.90       0.          0.
tortx      diff0      texp       beta       bknud
0.25       2.14  e-05 2.334e-00 0.          0.0     e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
   12      0.55   e-4 0.13       1.         .0018      1.    e-11 1.         0.8
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    8      0.4438     8.01  e-02 5.792e-07 5.0  e+08 1.0       1.0    e-04
intmin     intmax
-12.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.   e-11 1.    e-2 1.    e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
131600.    0.0        267.67     0.0        -69.5       0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.190e-17  phi0= 0.100e+00  rhor= 0.248e+04    cr= 0.840e+03
 rkml= 0.234e+01  rkmv= 0.190e+01   com= 0.        expan= 0.
tortx= 0.250e+00 diff0= 0.214e-04  texp= 0.233e+01
 beta= 0.        bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
 12  0.5500e-04 0.1300e+00 0.1000e+01 0.1800e-02 0.1000e-10 0.1000e+01
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  8  0.4438e+00 0.8010e-01 0.5792e-06 0.5000e+09 0.1000e+01 0.1000e-03

   Slr=0.1300e+00 Sltest=0.1300e+00   krl=0.1570e-09   krg=0.1000e+01
   pc2=-.1537e+10  denom=0.2412e+00

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           S0           Pa0
       0.100000e+06 0.300000e+00 0.973968e+05
       T0           Xga          Xla
       0.220000e+02 0.983627e+00 0.156700e-04

Integration Parameters
----------------------
etamin=0.6144e-05 etamax=0.6738e-02     zL=  -12.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.              Qe=0.              P=0.         T or S=0.
    Qa=0.              Pa=0.
 nzsav= 200        dzsav=0.3500e-01   ibat=0 ifxl=2 ifx2=3 ivpl= 1 idel= 1

 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1316e+06  0.2677e+03  -.6950e+02
 new  v=0.          0.          0.
 old   zL= -12.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -12.000, iph=3
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1316e+06  T= 267.6700
Sg=0.9142e+00 Pa=0.6554e-30 Xg=0.7975e-35 Xl=0.1055e-39
        ODEINT done,    zU=  -5.000, iph=3  , nok=278, nbad= 26
Qw=0.2438e-09 Qe=0.4112e-02 Qa=0.1402e-07  P=0.9997e+05  T=  22.0357
Sg=0.3002e+00 Pa=0.9736e+05 Xg=0.9836e+00 Xl=0.1566e-04
Converged

ith= 2
 old  v=0.1316e+06  0.2677e+03  -.6950e+02
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.5862e+01 seconds

 _________
|         |
|  Shoot  |
|_________|

-------------------------------------------------------------------
Starting values for shot  1
   v=0.1316e+06  0.2677e+03  -.6950e+02
delv=0.1316e+04  0.2677e+01  -.6950e+00   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
1
Stop
```

Sample problem 5 output file.

Problem 6: Enhanced vapor diffusion (input, output, and partial plot files shown)

Enhanced vapor diffusion (BETA=1) is added to problem 2, and the problem 2 converged values of V are used for initial guesses (see input file). A preshot indicates that shooting with these values has a reasonable chance of working (see output file), and shooting does in fact converge in four shots. As in problem 2, the number of shots needed for convergence could be decreased by using 'nudged' initial guesses based on the preshot results.

Sample problem 6 input file.

```
 ifx1 ifx2   nz ibat ivpl ilog idel
    2    0  200    0    0    1    1
qmw0       qma0       qe0        P0         T0/S0      Pa0/Xga0/Xla0/ln(Pa0)/T0
0.         0.         0667.67    100000.    .2         .979376 e5
perm       phi        rhor       cr         rkml       rkmv       com        expan
20.   e-15 0.10       2550.      800.       2.         2.         0.          0.
tortx      diff0      texp       beta       bknud
0.50       2.6   e-05 1.    e-10 1.        0.0      e5
  irp      rp(1)      rp(2)      rp(3)      rp(4)      rp(5)      rp(6)      rp(7)
    7      0.45       9.6   e-04 1.0
  icp      cp(1)      cp(2)      cp(3)      cp(4)      cp(5)      cp(6)      cp(7)
    7      0.45       1.0   e-03 8.    e-05 5.0   e+08 1.0
intmin     intmax
-11.0       -5.
eps(1e-5) hmin(sma) dv0        f0         tiny(det. for computer)
1.     e-4 1.    e-11 1.     e-2 1.     e-2
qwscale    qescale    pscale     tscale     qascale    pascale
0.         0.         0.         0.         0.         0.
v(1)       delv(1)    v(2)       delv(2)    v(3)       delv(3)
115100.    0.0        239.48     0.0        -43.72     0.0
```

```
SIMSOL OUTPUT
=============

Material Properties
-------------------
 perm= 0.200e-13  phi0= 0.100e+00  rhor= 0.255e+04    cr= 0.800e+03
 rkml= 0.200e+01  rkmv= 0.200e+01   com= 0.        expan= 0.
tortx= 0.500e+00 diff0= 0.260e-04  texp= 0.100e-09
 beta= 0.100e+01 bknud= 0.

Characteristic Curves
---------------------
irp    rp(1)       rp(2)       rp(3)       rp(4)       rp(5)       rp(6)
  7  0.4500e+00 0.9600e-03 0.1000e+01 0.          0.          0.
icp    cp(1)       cp(2)       cp(3)       cp(4)       cp(5)       cp(6)
  7  0.4500e+00 0.1000e-02 0.8000e-04 0.5000e+09 0.1000e+01 0.

   Slr=0.9600e-03 Sltest=0.1264e-02   krl=0.8350e-18   krg=0.1000e+01
   pc2=-.1306e+13  denom=0.1090e-05

Boundary Conditions
-------------------
zL:    Qw0          Qa0          Qe0
       0.           0.           0.667670e+03
zU:    P0           S0           Pa0
       0.100000e+06 0.200000e+00 0.979376e+05
       T0           Xga          Xla
       0.180003e+02 0.987057e+00 0.157570e-04

Integration Parameters
----------------------
etamin=0.1670e-04 etamax=0.6738e-02     zL=  -11.0000     zU=   -5.0000
   eps= 0.100e-03   hmin= 0.100e-10    dv0= 0.100e-01     f0= 0.100e-01
  tiny= 0.100e-13
Scaling factors
    Qw=0.              Qe=0.              P=0.         T or S=0.
    Qa=0.              Pa=0.
 nzsav= 200        dzsav=0.3000e-01   ibat=0 ifxl=2 ifx2=0 ivpl= 0 idel= 1

 __________
|          |
| Preshoot |
|__________|


ith= 1
 old  v=0.1151e+06  0.2395e+03  -.4372e+02
 new  v=0.          0.          0.
 old   zL= -11.000  zU=  -5.000  eps=0.10e-03
 new   zL=   0.000  zU=   0.000  eps=0.

        ODEINT started, zL= -11.000, iph=1
Qw=0.         Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 239.4800
Sg=0.1000e+01 Pa=0.1030e-18 Xg=0.1432e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3  , nok=179, nbad= 12
Qw=0.8181e-07 Qe=0.1530e-01 Qa=0.1173e-07  P=0.1001e+06  T=  35.3346
Sg=0.1414e+00 Pa=0.9437e+05 Xg=0.9636e+00 Xl=0.1518e-04

ith= 2
 old  v=0.1151e+06  0.2395e+03  -.4372e+02
 new  v=-.1000e+01  0.          0.
Elapsed CPU time after Preshooting=0.2561e+01 seconds

 _________
|         |
|  Shoot  |
|_________|

-----------------------------------------------------------------------
Starting values for shot  1
   v=0.1151e+06  0.2395e+03  -.4372e+02
delv=0.1151e+04  0.2395e+01  -.4372e+00   eps=0.10e-03
Continue with these parameters (0), stop (1),
read new parameters (2), or go back to preshooting (3)
0
Continue interactively (0) or switch to batch mode (1)
1
```

Sample problem 6 output file.

```
Main    ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 239.4800
Sg=0.1000e+01 Pa=0.1030e-18 Xg=0.1432e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=179, nbad= 12
Qw=0.8181e-07 Qe=0.1530e-01 Qa=0.1173e-07  P=0.1001e+06  T=  35.3346
Sg=0.1414e+00 Pa=0.9437e+05 Xg=0.9636e+00 Xl=0.1518e-04

Delv(1) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1163e+06  T= 239.4800
Sg=0.1000e+01 Pa=0.1030e-18 Xg=0.1418e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=174, nbad= 13
Qw=0.8021e-07 Qe=0.1503e-01 Qa=0.1180e-07  P=0.1015e+06  T=  35.2617
Sg=0.1417e+00 Pa=0.9580e+05 Xg=0.9642e+00 Xl=0.1541e-04

Delv(2) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 241.8748
Sg=0.1000e+01 Pa=0.1030e-18 Xg=0.1432e-23 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=177, nbad= 12
Qw=0.9156e-07 Qe=0.1780e-01 Qa=0.1230e-07  P=0.1001e+06  T=  37.2850
Sg=0.1433e+00 Pa=0.9373e+05 Xg=0.9593e+00 Xl=0.1508e-04

Delv(3) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1151e+06  T= 239.4800
Sg=0.1000e+01 Pa=0.6649e-19 Xg=0.9247e-24 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=180, nbad= 13
Qw=0.8411e-07 Qe=0.1565e-01 Qa=0.1167e-07  P=0.1000e+06  T=  35.3904
Sg=0.1400e+00 Pa=0.9429e+05 Xg=0.9634e+00 Xl=0.1517e-04

Shot  1 results
vL=0.1151e+06  vU=0.1001e+06  dv/vcrit=-.2379e+01  f/fcrit=0.9888e-01
vL=0.2395e+03  vU=0.1414e+00  dv/vcrit=-.4657e+01  f/fcrit=-.2930e+02
vL=-.4372e+02  vU=0.9437e+05  dv/vcrit=-.9186e+02  f/fcrit=-.3640e+01
-----------------------------------------------------------------------
Starting values for shot  2
   v=0.1124e+06  0.2288e+03  -.2279e+02
delv=0.1124e+04  0.2288e+01  -.2279e+00   eps=0.10e-03

Main    ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1124e+06  T= 228.8239
Sg=0.1000e+01 Pa=0.1269e-09 Xg=0.1806e-14 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=137, nbad= 14
Qw=0.2266e-07 Qe=0.4549e-02 Qa=0.1175e-07  P=0.1012e+06  T=  22.6241
Sg=0.2044e+00 Pa=0.9843e+05 Xg=0.9829e+00 Xl=0.1584e-04

Delv(1) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1135e+06  T= 228.8239
Sg=0.1000e+01 Pa=0.1269e-09 Xg=0.1788e-14 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=127, nbad= 13
Qw=0.2244e-07 Qe=0.4532e-02 Qa=0.1184e-07  P=0.1024e+06  T=  22.6053
Sg=0.2048e+00 Pa=0.9969e+05 Xg=0.9832e+00 Xl=0.1604e-04

Delv(2) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1124e+06  T= 231.1122
Sg=0.1000e+01 Pa=0.1269e-09 Xg=0.1806e-14 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=126, nbad= 14
Qw=0.2470e-07 Qe=0.5118e-02 Qa=0.1223e-07  P=0.1012e+06  T=  24.5283
Sg=0.2057e+00 Pa=0.9817e+05 Xg=0.9808e+00 Xl=0.1579e-04

Delv(3) ODEINT started, zL= -11.000, iph=1
Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1124e+06  T= 228.8239
Sg=0.1000e+01 Pa=0.1010e-09 Xg=0.1438e-14 Xl=0.
        ODEINT done,    zU=  -5.000, iph=3, nok=137, nbad= 15
Qw=0.2283e-07 Qe=0.4568e-02 Qa=0.1172e-07  P=0.1011e+06  T=  22.6751
Sg=0.2035e+00 Pa=0.9837e+05 Xg=0.9829e+00 Xl=0.1583e-04

Shot  2 results
vL=0.1124e+06  vU=0.1012e+06  dv/vcrit=-.7509e+00  f/fcrit=0.1171e+01
vL=0.2288e+03  vU=0.2044e+00  dv/vcrit=-.2129e+01  f/fcrit=0.2181e+01
vL=-.2279e+02  vU=0.9843e+05  dv/vcrit=0.1308e+01  f/fcrit=0.4988e+00
-----------------------------------------------------------------------
```

Sample problem 6 output file (continued).

```
Starting values for shot  3
    v=0.1116e+06  0.2241e+03  -.2309e+02
 delv=0.1116e+04  0.2241e+01  -.2309e+00   eps=0.10e-03

 Main    ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1116e+06  T= 224.0535
 Sg=0.1000e+01 Pa=0.9380e-10 Xg=0.1345e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=133, nbad= 13
 Qw=0.1915e-07 Qe=0.3534e-02 Qa=0.1062e-07  P=0.1002e+06  T=  18.5049
 Sg=0.1983e+00 Pa=0.9808e+05 Xg=0.9867e+00 Xl=0.1578e-04
 All f < fcrit

 Delv(1) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1127e+06  T= 224.0535
 Sg=0.1000e+01 Pa=0.9380e-10 Xg=0.1332e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=129, nbad= 13
 Qw=0.1897e-07 Qe=0.3524e-02 Qa=0.1071e-07  P=0.1015e+06  T=  18.4864
 Sg=0.1989e+00 Pa=0.9933e+05 Xg=0.9868e+00 Xl=0.1598e-04

 Delv(2) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1116e+06  T= 226.2940
 Sg=0.1000e+01 Pa=0.9380e-10 Xg=0.1345e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=140, nbad= 15
 Qw=0.2092e-07 Qe=0.3994e-02 Qa=0.1108e-07  P=0.1002e+06  T=  20.4735
 Sg=0.2003e+00 Pa=0.9780e+05 Xg=0.9849e+00 Xl=0.1573e-04

 Delv(3) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1116e+06  T= 224.0535
 Sg=0.1000e+01 Pa=0.7446e-10 Xg=0.1068e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=135, nbad= 11
 Qw=0.1930e-07 Qe=0.3547e-02 Qa=0.1059e-07  P=0.1002e+06  T=  18.5570
 Sg=0.1975e+00 Pa=0.9802e+05 Xg=0.9866e+00 Xl=0.1577e-04

 Shot  3 results
 vL=0.1116e+06  vU=0.1002e+06  dv/vcrit=-.2798e+00  f/fcrit=0.2120e+00
 vL=0.2241e+03  vU=0.1983e+00  dv/vcrit=-.1787e+00  f/fcrit=-.8316e+00
 vL=-.2309e+02  vU=0.9808e+05  dv/vcrit=-.2597e+01  f/fcrit=0.1487e+00
 ---------------------------------------------------------------------
 Starting values for shot  4
    v=0.1113e+06  0.2237e+03  -.2251e+02
 delv=0.1113e+04  0.2237e+01  -.2251e+00   eps=0.10e-03

 Main    ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1113e+06  T= 223.6537
 Sg=0.1000e+01 Pa=0.1683e-09 Xg=0.2420e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=128, nbad= 12
 Qw=0.1854e-07 Qe=0.3416e-02 Qa=0.1055e-07  P=0.1001e+06  T=  17.9667
 Sg=0.1995e+00 Pa=0.9801e+05 Xg=0.9871e+00 Xl=0.1577e-04
 All f < fcrit

 Delv(1) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1124e+06  T= 223.6537
 Sg=0.1000e+01 Pa=0.1683e-09 Xg=0.2396e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=127, nbad= 12
 Qw=0.1837e-07 Qe=0.3405e-02 Qa=0.1063e-07  P=0.1013e+06  T=  17.9387
 Sg=0.1999e+00 Pa=0.9926e+05 Xg=0.9873e+00 Xl=0.1597e-04

 Delv(2) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1113e+06  T= 225.8903
 Sg=0.1000e+01 Pa=0.1683e-09 Xg=0.2420e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=129, nbad= 14
 Qw=0.2025e-07 Qe=0.3868e-02 Qa=0.1103e-07  P=0.1000e+06  T=  19.9701
 Sg=0.2018e+00 Pa=0.9768e+05 Xg=0.9853e+00 Xl=0.1572e-04

 Delv(3) ODEINT started, zL= -11.000, iph=1
 Qw=0.          Qe=0.1063e+03 Qa=0.          P=0.1113e+06  T= 223.6537
 Sg=0.1000e+01 Pa=0.1344e-09 Xg=0.1932e-14 Xl=0.
         ODEINT done,    zU=  -5.000, iph=3, nok=128, nbad= 13
 Qw=0.1868e-07 Qe=0.3428e-02 Qa=0.1052e-07  P=0.1000e+06  T=  18.0181
 Sg=0.1986e+00 Pa=0.9795e+05 Xg=0.9870e+00 Xl=0.1576e-04

 Shot  4 results
 vL=0.1113e+06  vU=0.1001e+06  dv/vcrit=-.7531e-01  f/fcrit=0.6401e-01
 vL=0.2237e+03  vU=0.1995e+00  dv/vcrit=0.2959e-01  f/fcrit=-.2718e+00
 vL=-.2251e+02  vU=0.9801e+05  dv/vcrit=-.6111e+00  f/fcrit=0.6980e-01

 Converged, is= 4 CPU time=  29.778 seconds
```

Sample problem 6 output file (continued).

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
aa 10	-11.00000	0.	667.6700	1.15100	239.48000	0.	1	1	2
aa 10	-10.90040	0.5032e-12	667.6606	1.15100	234.18800	.1032e-59	4	1	1
aa 10	-10.68651	0.2045e-11	667.6327	1.15100	222.82420	.4192e-59	5	1	1
aa 10	-10.40710	0.5558e-11	667.5728	1.15100	207.98020	.1139e-58	6	1	1
aa 10	-10.10358	0.1290e-10	667.4561	1.15100	191.85710	.2645e-58	7	1	1
aa 10	-9.78938	0.2814e-10	667.2317	1.15100	175.17150	.5770e-58	8	1	1
aa 10	-9.47128	0.5970e-10	666.8042	1.15100	158.28630	.1224e-57	9	1	1
aa 10	-9.15267	0.1249e-09	665.9955	1.15100	141.38920	.2561e-57	10	1	1
aa 10	-8.83554	0.2593e-09	664.4783	1.15100	124.59890	.5316e-57	11	1	1
aa 10	-8.52057	0.5361e-09	661.6531	1.15100	107.97570	.1099e-56	12	1	1
aa 10	-8.43759	0.6494e-09	660.5651	1.15100	103.61000	.1331e-56	0	1	0
aa 10	-8.43759	0.6494e-09	660.5651	1.15100	103.61000	.1331e-56	13	3	1
aa 10	-8.40394	0.5069e-05	662.6682	1.13911	103.31290	.9244e-31	35	3	6
aa 10	-8.37022	0.6220e-05	663.0657	1.12711	103.01040	.1716e-29	42	3	6
aa 10	-8.33983	0.7026e-05	663.3146	1.11622	102.73360	.2841e-28	49	3	6
aa 10	-8.30792	0.7787e-05	663.5292	1.10469	102.43830	.6977e-27	57	3	6
aa 10	-8.27487	0.8545e-05	663.7265	1.09265	102.12690	.2554e-25	66	3	6
aa 10	-8.24437	0.9247e-05	663.8984	1.08143	101.83440	.9324e-24	75	3	6
aa 10	-8.21311	0.9992e-05	664.0720	1.06982	101.52880	.5056e-22	85	3	6
aa 10	-8.18163	0.1078e-04	664.2499	1.05798	101.21450	.4065e-20	96	3	6
aa 10	-8.15044	0.1162e-04	664.4337	1.04609	100.89570	.4836e-18	108	3	6
aa 10	-8.12008	0.1251e-04	664.6233	1.03431	100.57720	.8501e-16	121	3	6
aa 10	-8.08910	0.1349e-04	664.8300	1.02205	100.24220	.3276e-13	136	3	6
aa 10	-8.05775	0.1448e-04	664.9830	1.01052	99.84560	.1728e-10	152	3	6
aa 10	-8.01749	0.1493e-04	664.5046	1.00647	98.91240	.1916e-09	158	3	5
aa 10	-7.96880	0.1519e-04	663.6107	1.00509	97.62680	.4577e-09	160	3	5
aa 10	-7.92308	0.1539e-04	662.6141	1.00438	96.36690	.7276e-09	161	3	5
aa 10	-7.85057	0.1569e-04	660.7313	1.00366	94.29150	.1190e-08	162	3	5
aa 10	-7.73432	0.1618e-04	656.8277	1.00296	90.79060	.2018e-08	163	3	5
aa 10	-7.54982	0.1707e-04	647.6877	1.00229	84.83890	.3575e-08	164	3	5
aa 10	-7.27674	0.1872e-04	624.0357	1.00174	75.30430	.6507e-08	165	3	5
aa 10	-6.94468	0.2136e-04	567.9477	1.00140	63.14050	.1131e-07	166	3	6
aa 10	-6.65686	0.2393e-04	481.6730	1.00125	53.05240	.1702e-07	167	3	1
aa 10	-6.39443	0.2553e-04	366.4236	1.00117	45.25770	.2426e-07	168	3	5
aa 10	-6.18873	0.2517e-04	258.2346	1.00113	40.66720	.3195e-07	169	3	1
aa 10	-6.03331	0.2328e-04	176.1554	1.00111	38.24420	.3913e-07	170	3	1
aa 10	-5.91317	0.2070e-04	119.2239	1.00110	36.97270	.4535e-07	171	3	2
aa 10	-5.81617	0.1795e-04	80.6181	1.00108	36.28170	.5060e-07	172	3	2
aa 10	-5.73322	0.1525e-04	54.0626	1.00108	35.88650	.5504e-07	173	3	2
aa 10	-5.66220	0.1281e-04	36.3311	1.00107	35.66160	.5868e-07	174	3	2
aa 10	-5.59941	0.1065e-04	24.3636	1.00106	35.52960	.6167e-07	175	3	2
aa 10	-5.54347	0.8794e-05	16.3621	1.00105	35.45190	.6410e-07	176	3	2
aa 10	-5.48730	0.7064e-05	10.5049	1.00105	35.40160	.6627e-07	177	3	2
aa 10	-5.44171	0.5791e-05	7.0876	1.00104	35.37530	.6781e-07	178	3	2
aa 10	-5.39611	0.4656e-05	4.6334	1.00104	35.35840	.6914e-07	179	3	2
aa 10	-5.35439	0.3750e-05	3.0556	1.00103	35.34860	.7018e-07	180	3	2
aa 10	-5.31576	0.3026e-05	2.0327	1.00103	35.34280	.7100e-07	181	3	2
aa 10	-5.28008	0.2456e-05	1.3720	1.00102	35.33950	.7163e-07	182	3	2
aa 10	-5.24626	0.2000e-05	0.9348	1.00102	35.33750	.7213e-07	183	3	2
aa 10	-5.21491	0.1645e-05	0.6519	1.00102	35.33630	.7251e-07	184	3	2
aa 10	-5.18487	0.1363e-05	0.4624	1.00101	35.33560	.7281e-07	185	3	2
aa 10	-5.12837	0.9623e-06	0.2504	1.00100	35.33490	.7323e-07	187	3	2
aa 10	-5.07537	0.7147e-06	0.1537	1.00100	35.33470	.7349e-07	189	3	2
aa 10	-5.02366	0.5620e-06	0.1081	1.00099	35.33460	.7363e-07	191	3	2
aa 10	-5.00000	0.5140e-06	0.0961	1.00099	35.33460	.7368e-07	192	3	2

Sample problem 6 plot file (first shot).

Label	z	$\ln(P_a)$ (bars)	S_g	Q_g (kg/s/m)	Q_l (kg/s/m)	X_g^a	NSTP	IPH	IERR
bb 10	-11.00000	-.5523e+020	.1000e+010	.	0.	0.1432e-23	1	1	2
bb 10	-10.90040	-.5523e+020	.1000e+010	.5032e-120	.	0.1432e-23	4	1	1
bb 10	-10.68651	-.5523e+020	.1000e+010	.2045e-110	.	0.1432e-23	5	1	1
bb 10	-10.40710	-.5523e+020	.1000e+010	.5558e-110	.	0.1432e-23	6	1	1
bb 10	-10.10358	-.5523e+020	.1000e+010	.1290e-100	.	0.1432e-23	7	1	1
bb 10	-9.78938	-.5523e+020	.1000e+010	.2814e-100	.	0.1432e-23	8	1	1
bb 10	-9.47128	-.5523e+020	.1000e+010	.5970e-100	.	0.1432e-23	9	1	1
bb 10	-9.15267	-.5523e+020	.1000e+010	.1249e-090	.	0.1432e-23	10	1	1
bb 10	-8.83554	-.5522e+020	.1000e+010	.2593e-090	.	0.1432e-23	11	1	1
bb 10	-8.52057	-.5522e+020	.1000e+010	.5361e-090	.	0.1432e-23	12	1	1
bb 10	-8.43759	-.5522e+020	.1000e+010	.6494e-090	.	0.1432e-23	0	1	0
bb 10	-8.43759	-.5522e+020	.9987e+000	.2449e-03	-.2449e-03	0.1432e-23	13	3	1
bb 10	-8.40394	-.5282e+020	.6436e+000	.2441e-03	-.2390e-03	0.1602e-22	35	3	6
bb 10	-8.37022	-.4998e+020	.5696e+000	.2431e-03	-.2369e-03	0.2761e-21	42	3	6
bb 10	-8.33983	-.4716e+020	.5211e+000	.2422e-03	-.2352e-03	0.4682e-20	49	3	6
bb 10	-8.30792	-.4394e+020	.4782e+000	.2412e-03	-.2335e-03	0.1181e-18	57	3	6
bb 10	-8.27487	-.4032e+020	.4381e+000	.2401e-03	-.2316e-03	0.4442e-17	66	3	6
bb 10	-8.24437	-.3671e+020	.4033e+000	.2390e-03	-.2298e-03	0.1666e-15	75	3	6
bb 10	-8.21311	-.3270e+020	.3686e+000	.2378e-03	-.2278e-03	0.9330e-14	85	3	6
bb 10	-8.18163	-.2828e+020	.3340e+000	.2364e-03	-.2256e-03	0.7808e-12	96	3	6
bb 10	-8.15044	-.2346e+020	.2996e+000	.2348e-03	-.2232e-03	0.9769e-10	108	3	6
bb 10	-8.12008	-.1824e+020	.2655e+000	.2331e-03	-.2206e-03	0.1828e-07	121	3	6
bb 10	-8.08910	-.1222e+020	.2298e+000	.2308e-03	-.2173e-03	0.7652e-05	136	3	6
bb 10	-8.05775	-.5864e+010	.1961e+000	.1930e-03	-.1785e-03	0.4439e-02	152	3	6
bb 10	-8.01749	-.3444e+010	.1823e+000	.1494e-03	-.1345e-03	0.4931e-01	158	3	5
bb 10	-7.96880	-.2594e+010	.1755e+000	.1401e-03	-.1249e-03	0.1128e+00	160	3	5
bb 10	-7.92308	-.2157e+010	.1710e+000	.1344e-03	-.1190e-03	0.1710e+00	161	3	5
bb 10	-7.85057	-.1714e+010	.1652e+000	.1265e-03	-.1108e-03	0.2576e+00	162	3	5
bb 10	-7.73432	-.1271e+010	.1577e+000	.1146e-03	-.9837e-04	0.3814e+00	163	3	5
bb 10	-7.54982	-.8489e+000	.1485e+000	.9629e-04	-.7922e-04	0.5423e+00	164	3	5
bb 10	-7.27674	-.4921e+000	.1390e+000	.7082e-04	-.5210e-04	0.7140e+00	165	3	5
bb 10	-6.94468	-.2596e+000	.1321e+000	.4416e-04	-.2279e-04	0.8428e+00	166	3	6
bb 10	-6.65686	-.1532e+000	.1298e+000	.2644e-04	-.2495e-05	0.9055e+00	167	3	1
bb 10	-6.39443	-.1008e+000	.1304e+000	.1499e-04	0.1056e-04	0.9372e+00	168	3	5
bb 10	-6.18873	-.7827e-010	.1323e+000	.8788e-05	0.1641e-04	0.9510e+00	169	3	1
bb 10	-6.03331	-.6829e-010	.1343e+000	.5420e-05	0.1790e-04	0.9571e+00	170	3	1
bb 10	-5.91317	-.6353e-010	.1360e+000	.3478e-05	0.1727e-04	0.9600e+00	171	3	2
bb 10	-5.81617	-.6107e-010	.1373e+000	.2289e-05	0.1571e-04	0.9616e+00	172	3	2
bb 10	-5.73322	-.5970e-010	.1383e+000	.1518e-05	0.1378e-04	0.9624e+00	173	3	2
bb 10	-5.66220	-.5894e-010	.1391e+000	.1023e-05	0.1184e-04	0.9629e+00	174	3	2
bb 10	-5.59941	-.5850e-010	.1397e+000	.6966e-06	0.1001e-04	0.9632e+00	175	3	2
bb 10	-5.54347	-.5825e-010	.1401e+000	.4828e-06	0.8375e-05	0.9633e+00	176	3	2
bb 10	-5.48730	-.5808e-010	.1405e+000	.3293e-06	0.6801e-05	0.9634e+00	177	3	2
bb 10	-5.44171	-.5800e-010	.1407e+000	.2413e-06	0.5618e-05	0.9635e+00	178	3	2
bb 10	-5.39611	-.5795e-010	.1409e+000	.1795e-06	0.4546e-05	0.9635e+00	179	3	2
bb 10	-5.35439	-.5792e-010	.1410e+000	.1407e-06	0.3679e-05	0.9635e+00	180	3	2
bb 10	-5.31576	-.5791e-010	.1411e+000	.1162e-06	0.2981e-05	0.9635e+00	181	3	2
bb 10	-5.28008	-.5790e-010	.1412e+000	.1010e-06	0.2427e-05	0.9635e+00	182	3	2
bb 10	-5.24626	-.5790e-010	.1413e+000	.9128e-07	0.1981e-05	0.9635e+00	183	3	2
bb 10	-5.21491	-.5790e-010	.1413e+000	.8532e-07	0.1633e-05	0.9635e+00	184	3	2
bb 10	-5.18487	-.5790e-010	.1413e+000	.8156e-07	0.1354e-05	0.9636e+00	185	3	2
bb 10	-5.12837	-.5791e-010	.1414e+000	.7778e-07	0.9577e-06	0.9636e+00	187	3	2
bb 10	-5.07537	-.5791e-010	.1414e+000	.7638e-07	0.7118e-06	0.9636e+00	189	3	2
bb 10	-5.02366	-.5792e-010	.1414e+000	.7590e-07	0.5597e-06	0.9636e+00	191	3	2
bb 10	-5.00000	-.5792e-010	.1414e+000	.7585e-07	0.5344e-06	0.9636e+00	192	3	2

Sample problem 6 plot file (first shot).

Label	z	Q_w (kg/s/m)	Q_e (W/m)	P (bars)	T°C	Q_a (kg/s/m)	NSTP	IPH	IERR
aa 40	-11.000000.		667.6700	1.11276	223.65370.		1	1	2
aa 40	-10.899800	.5230e-12	667.6605	1.11276	218.32970	.3062e-41	4	1	1
aa 40	-10.702400	.1967e-11	667.6352	1.11276	207.84200	.1152e-40	5	1	1
aa 40	-10.427240	.5409e-11	667.5784	1.11276	193.22400	.3167e-40	6	1	1
aa 40	-10.125910	.1263e-10	667.4673	1.11276	177.21710	.7396e-40	7	1	1
aa 40	-9.813860	.2761e-10	667.2546	1.11276	160.64490	.1616e-39	8	1	1
aa 40	-9.498260	.5854e-10	666.8518	1.11276	143.89150	.3427e-39	9	1	1
aa 40	-9.182280	.1224e-09	666.0941	1.11276	127.13190	.7164e-39	10	1	1
aa 40	-8.867980	.2537e-09	664.6810	1.11276	110.48800	.1485e-38	11	1	1
aa 40	-8.719590	.3581e-09	663.6368	1.11276	102.64520	.2096e-38	0	1	0
aa 40	-8.719590	.3581e-09	663.6368	1.11276	102.64520	.2096e-38	12	3	1
aa 40	-8.685480	.2947e-05	664.8455	1.10042	102.32820	.9107e-22	31	3	5
aa 40	-8.652150	.3579e-05	665.0568	1.08828	102.01330	.1637e-20	38	3	5
aa 40	-8.621770	.4036e-05	665.1925	1.07713	101.72160	.2707e-19	45	3	6
aa 40	-8.589880	.4470e-05	665.3099	1.06534	101.41020	.6644e-18	53	3	6
aa 40	-8.556880	.4906e-05	665.4180	1.05302	101.08200	.2429e-16	62	3	6
aa 40	-8.526470	.5311e-05	665.5122	1.04156	100.77380	.8855e-15	71	3	6
aa 40	-8.495360	.5740e-05	665.6073	1.02972	100.45180	.4792e-13	81	3	6
aa 40	-8.463400	.6198e-05	665.6985	1.01772	100.09950	.3759e-11	92	3	6
aa 40	-8.432600	.6510e-05	665.6629	1.01072	99.55810	.5715e-10	99	3	5
aa 40	-8.391230	.6722e-05	665.4190	1.00770	98.55200	.1972e-09	102	3	5
aa 40	-8.321680	.6977e-05	664.8331	1.00565	96.68260	.4748e-09	104	3	5
aa 40	-8.256420	.7195e-05	664.1344	1.00462	94.82670	.7602e-09	105	3	5
aa 40	-8.152870	.7539e-05	662.7070	1.00360	91.72390	.1256e-08	106	3	5
aa 40	-7.989000	.8124e-05	659.4355	1.00262	86.45430	.2155e-08	107	3	5
aa 40	-7.749340	.9135e-05	651.3426	1.00182	78.02930	.3747e-08	108	3	5
aa 40	-7.466530	.1065e-04	633.3544	1.00131	67.18720	.6122e-08	109	3	5
aa 40	-7.185800	.1253e-04	599.9845	1.00104	55.86610	.9163e-08	110	3	1
aa 40	-6.967990	.1413e-04	557.4824	1.00092	47.11300	.1223e-07	111	3	1
aa 40	-6.767350	.1544e-04	500.8927	1.00085	39.45980	.1596e-07	112	3	1
aa 40	-6.562820	.1612e-04	423.2550	1.00080	32.46580	.2125e-07	113	3	1
aa 40	-6.376750	.1553e-04	336.1432	1.00077	27.15200	.2793e-07	114	3	1
aa 40	-6.229820	.1391e-04	260.2088	1.00075	23.83100	.3469e-07	115	3	1
aa 40	-6.101310	.1162e-04	193.4474	1.00074	21.61350	.4147e-07	116	3	1
aa 40	-5.985400	.9057e-05	137.3419	1.00073	20.15360	.4784e-07	117	3	1
aa 40	-5.867850	.6342e-05	88.4796	1.00072	19.14520	.5392e-07	118	3	1
aa 40	-5.779950	.4482e-05	59.0785	1.00071	18.65210	.5783e-07	119	3	2
aa 40	-5.705200	.3138e-05	39.4354	1.00070	18.37230	.6055e-07	120	3	2
aa 40	-5.640140	.2189e-05	26.3128	1.00070	18.20990	.6243e-07	121	3	2
aa 40	-5.582220	.1527e-05	17.5102	1.00069	18.11360	.6371e-07	122	3	2
aa 40	-5.530200	.1072e-05	11.6426	1.00069	18.05610	.6459e-07	123	3	2
aa 40	-5.477840	.7321e-06	7.3806	1.00068	18.01850	.6523e-07	124	3	2
aa 40	-5.435430	.5319e-06	4.9207	1.00068	17.99880	.6560e-07	125	3	2
aa 40	-5.392630	.3856e-06	3.1535	1.00068	17.98570	.6587e-07	126	3	2
aa 40	-5.353140	.2903e-06	2.0216	1.00067	17.97810	.6604e-07	127	3	2
aa 40	-5.316780	.2289e-06	1.3021	1.00067	17.97350	.6615e-07	128	3	2
aa 40	-5.283170	.1894e-06	0.8439	1.00067	17.97090	.6622e-07	129	3	2
aa 40	-5.251940	.1638e-06	0.5511	1.00066	17.96920	.6626e-07	130	3	2
aa 40	-5.194980	.1364e-06	0.2404	1.00066	17.96770	.6629e-07	132	3	2
aa 40	-5.143550	.1246e-06	0.1099	1.00065	17.96710	.6630e-07	134	3	2
aa 40	-5.096910	.1197e-06	0.0555	1.00065	17.96690	.6630e-07	136	3	2
aa 40	-5.053300	.1176e-06	0.0326	1.00064	17.96680	.6629e-07	138	3	2
aa 40	-5.011260	.1167e-06	0.0229	1.00064	17.96670	.6628e-07	140	3	2
aa 40	-5.000000	.1165e-06	0.0215	1.00064	17.96670	.6628e-07	141	3	2

Sample problem 6 plot file (final shot).

Label	z	$\ln(P_a)$ (bars)	S_g	Q_g (kg/s/m)	Q_l (kg/s/m)	X_g^a	NSTP	IPH	IERR
bb 40	-11.00000	-.3402e+02	0.1000e+01	0.	0.	0.2420e-14	1	1	2
bb 40	-10.89980	-.3402e+02	0.1000e+01	0.5230e-12	0.	0.2420e-14	4	1	1
bb 40	-10.70240	-.3402e+02	0.1000e+01	0.1967e-11	0.	0.2420e-14	5	1	1
bb 40	-10.42724	-.3402e+02	0.1000e+01	0.5409e-11	0.	0.2420e-14	6	1	1
bb 40	-10.12591	-.3402e+02	0.1000e+01	0.1263e-10	0.	0.2420e-14	7	1	1
bb 40	-9.81386	-.3401e+02	0.1000e+01	0.2761e-10	0.	0.2420e-14	8	1	1
bb 40	-9.49826	-.3401e+02	0.1000e+01	0.5854e-10	0.	0.2420e-14	9	1	1
bb 40	-9.18228	-.3401e+02	0.1000e+01	0.1224e-09	0.	0.2420e-14	10	1	1
bb 40	-8.86798	-.3401e+02	0.1000e+01	0.2537e-09	0.	0.2420e-14	11	1	1
bb 40	-8.71959	-.3401e+02	0.1000e+01	0.3581e-09	0.	0.2420e-14	0	1	0
bb 40	-8.71959	-.3401e+02	0.9987e+00	0.2435e-03	-.2435e-03	0.2420e-14	12	3	1
bb 40	-8.68548	-.3154e+02	0.6356e+00	0.2425e-03	-.2396e-03	0.2877e-13	31	3	5
bb 40	-8.65215	-.2873e+02	0.5642e+00	0.2415e-03	-.2379e-03	0.4823e-12	38	3	5
bb 40	-8.62177	-.2591e+02	0.5160e+00	0.2406e-03	-.2365e-03	0.8184e-11	45	3	6
bb 40	-8.58988	-.2269e+02	0.4730e+00	0.2395e-03	-.2350e-03	0.2067e-09	53	3	6
bb 40	-8.55688	-.1908e+02	0.4326e+00	0.2383e-03	-.2334e-03	0.7782e-08	62	3	6
bb 40	-8.52647	-.1546e+02	0.3973e+00	0.2371e-03	-.2318e-03	0.2922e-06	71	3	6
bb 40	-8.49536	-.1145e+02	0.3622e+00	0.2356e-03	-.2299e-03	0.1639e-04	81	3	6
bb 40	-8.46340	-.7054e+01	0.3271e+00	0.2237e-03	-.2175e-03	0.1342e-02	92	3	6
bb 40	-8.43260	-.4316e+01	0.3047e+00	0.1711e-03	-.1646e-03	0.2075e-01	99	3	5
bb 40	-8.39123	-.3085e+01	0.2909e+00	0.1500e-03	-.1433e-03	0.6997e-01	102	3	5
bb 40	-8.32168	-.2238e+01	0.2765e+00	0.1381e-03	-.1311e-03	0.1582e+00	104	3	5
bb 40	-8.25642	-.1803e+01	0.2660e+00	0.1304e-03	-.1232e-03	0.2372e+00	105	3	5
bb 40	-8.15287	-.1365e+01	0.2524e+00	0.1195e-03	-.1119e-03	0.3513e+00	106	3	5
bb 40	-7.98900	-.9395e+00	0.2354e+00	0.1031e-03	-.9500e-04	0.5038e+00	107	3	5
bb 40	-7.74934	-.5713e+00	0.2170e+00	0.8049e-04	-.7135e-04	0.6731e+00	108	3	5
bb 40	-7.46653	-.3206e+00	0.2020e+00	0.5642e-04	-.4577e-04	0.8079e+00	109	3	5
bb 40	-7.18580	-.1780e+00	0.1928e+00	0.3664e-04	-.2410e-04	0.8909e+00	110	3	1
bb 40	-6.96799	-.1118e+00	0.1889e+00	0.2469e-04	-.1055e-04	0.9307e+00	111	3	1
bb 40	-6.76735	-.7344e-01	0.1875e+00	0.1637e-04	-.9180e-06	0.9541e+00	112	3	1
bb 40	-6.56282	-.4919e-01	0.1881e+00	0.1028e-04	0.5860e-05	0.9690e+00	113	3	1
bb 40	-6.37675	-.3582e-01	0.1901e+00	0.6432e-05	0.9128e-05	0.9773e+00	114	3	1
bb 40	-6.22982	-.2919e-01	0.1923e+00	0.4272e-05	0.9670e-05	0.9814e+00	115	3	1
bb 40	-6.10131	-.2538e-01	0.1944e+00	0.2871e-05	0.8788e-05	0.9838e+00	116	3	1
bb 40	-5.98540	-.2312e-01	0.1961e+00	0.1917e-05	0.7188e-05	0.9852e+00	117	3	1
bb 40	-5.86785	-.2167e-01	0.1975e+00	0.1199e-05	0.5197e-05	0.9861e+00	118	3	1
bb 40	-5.77995	-.2099e-01	0.1983e+00	0.8036e-06	0.3737e-05	0.9865e+00	119	3	2
bb 40	-5.70520	-.2062e-01	0.1987e+00	0.5515e-06	0.2647e-05	0.9868e+00	120	3	2
bb 40	-5.64014	-.2041e-01	0.1990e+00	0.3874e-06	0.1864e-05	0.9869e+00	121	3	2
bb 40	-5.58222	-.2028e-01	0.1992e+00	0.2791e-06	0.1312e-05	0.9870e+00	122	3	2
bb 40	-5.53020	-.2021e-01	0.1993e+00	0.2075e-06	0.9287e-06	0.9870e+00	123	3	2
bb 40	-5.47784	-.2017e-01	0.1994e+00	0.1558e-06	0.6416e-06	0.9871e+00	124	3	2
bb 40	-5.43543	-.2014e-01	0.1994e+00	0.1261e-06	0.4715e-06	0.9871e+00	125	3	2
bb 40	-5.39263	-.2013e-01	0.1994e+00	0.1047e-06	0.3467e-06	0.9871e+00	126	3	2
bb 40	-5.35314	-.2012e-01	0.1994e+00	0.9110e-07	0.2652e-06	0.9871e+00	127	3	2
bb 40	-5.31678	-.2012e-01	0.1994e+00	0.8244e-07	0.2126e-06	0.9871e+00	128	3	2
bb 40	-5.28317	-.2012e-01	0.1994e+00	0.7692e-07	0.1787e-06	0.9871e+00	129	3	2
bb 40	-5.25194	-.2012e-01	0.1995e+00	0.7340e-07	0.1567e-06	0.9871e+00	130	3	2
bb 40	-5.19498	-.2013e-01	0.1995e+00	0.6965e-07	0.1330e-06	0.9871e+00	132	3	2
bb 40	-5.14355	-.2013e-01	0.1995e+00	0.6807e-07	0.1229e-06	0.9871e+00	134	3	2
bb 40	-5.09691	-.2013e-01	0.1995e+00	0.6741e-07	0.1186e-06	0.9871e+00	136	3	2
bb 40	-5.05330	-.2014e-01	0.1995e+00	0.6712e-07	0.1167e-06	0.9871e+00	138	3	2
bb 40	-5.01126	-.2014e-01	0.1995e+00	0.6699e-07	0.1159e-06	0.9871e+00	140	3	2
bb 40	-5.00000	-.2014e-01	0.1995e+00	0.6698e-07	0.1159e-06	0.9871e+00	141	3	2

Sample problem 6 plot file (final shot).

V. ACKNOWLEDGEMENTS

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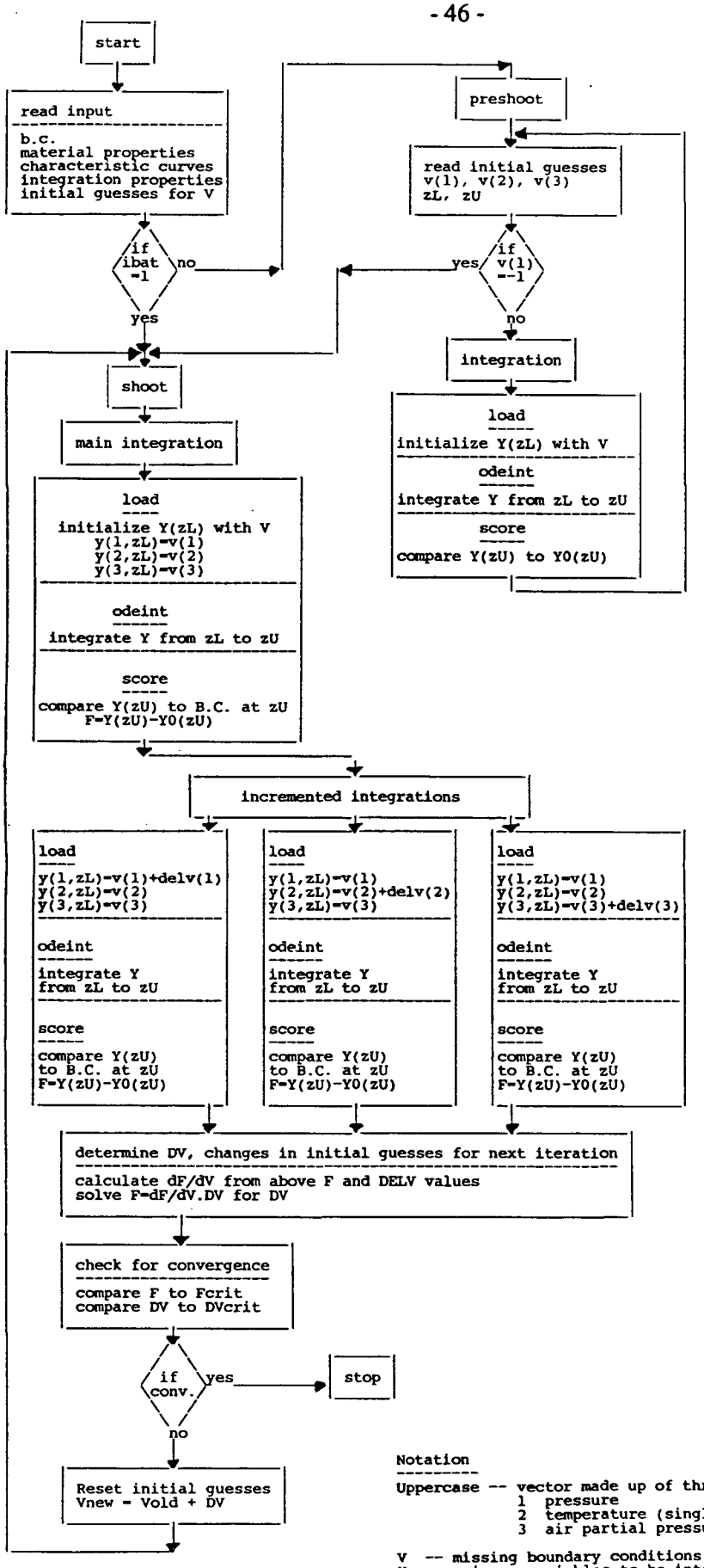

Figure 1. Flow chart for SIMSOL.

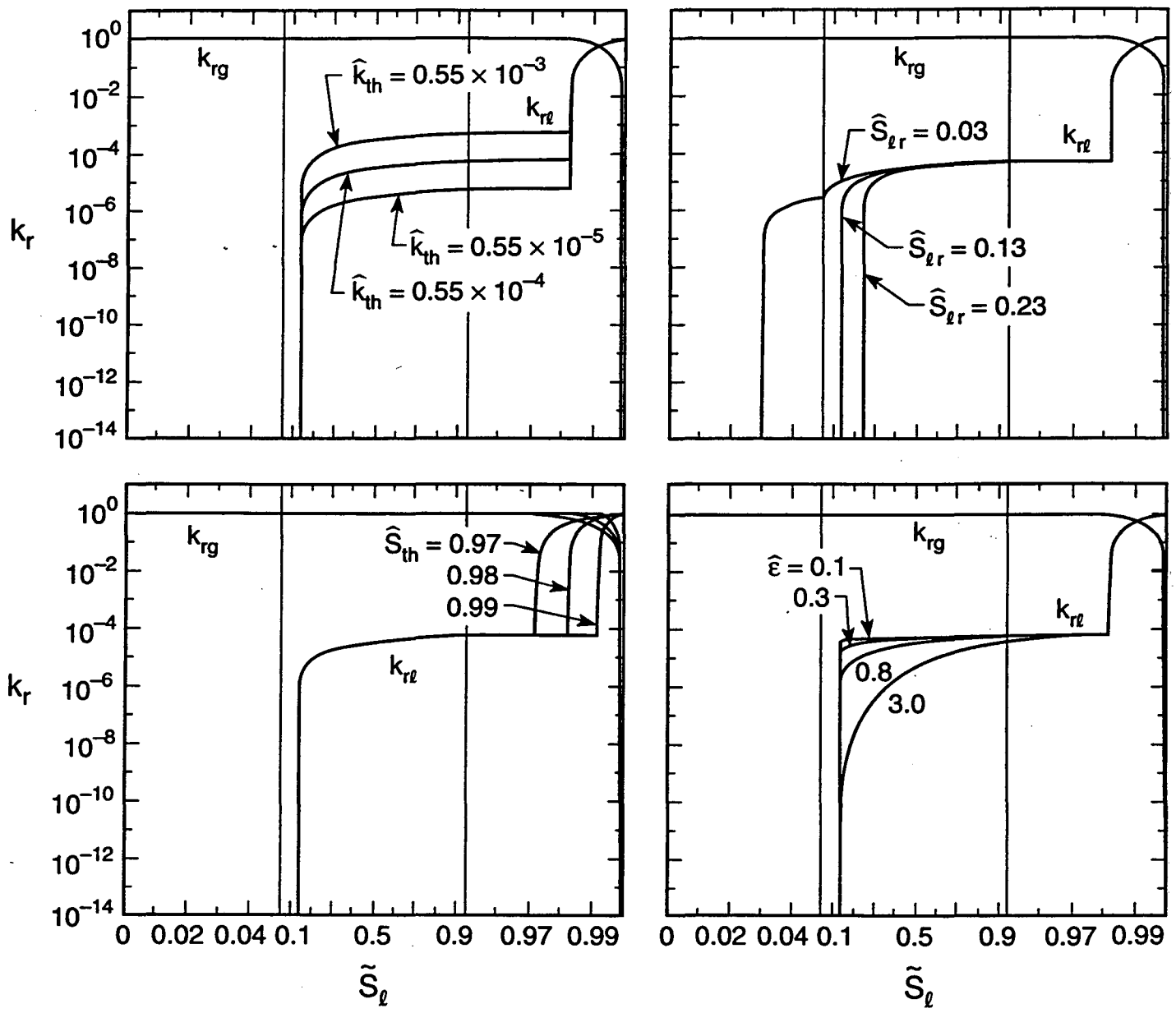

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Figure 2. Double-hump relative permeability curves illustrating the parameters used for IRP=12. The parameters $\hat{k}_{th}$, $\hat{S}_{lr}$, and $\hat{\varepsilon}$ are read in input item 4. The parameter $\hat{S}_{th}$ is calculated internally from the expression $\hat{S}_{th} = \phi_m V_m / (\phi_m V_m + \phi_f V_f)$, where ϕ_m is read in item 3, ϕ_f and V_f are read in item 4, and $V_m = 1 - V_f$.

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