A summary of the program execution is placed in the file *infile*.sum. Debugging information is placed in the file *infile*.dbg. In addition, ADEPT/F creates a file called *infile*.dat. which contains information about the internal variables (carrier concentrations, electric fields, recombination, etc.) at each operating point. This information can be displayed graphically using PLOTA, which is described later in this document.

The input file contains a series of 'cards' which may be of the following forms:

```
*titlecard anything at all
```

or

```
cardname var1=value1 var2=string2
+ array1=va1/va2/va3
```

The card name and continuation mark (+) must start in column 1. A 'card' can be up to 10 lines long. Any line starting with a blank or a $ is ignored. In the second example, assignment expressions cannot contain any embedded spaces. Assignment expressions must be be separated by a space, as shown above, or a comma.

The following tables describe the options and parameters which can be specified by the input file. Although the parameters are shown as uppercase, ADEPT/F treats uppercase and lowercase letters the same.

*TITLE

All characters following *TITLE (up to column 80) become part of a comment used to annotate the output.

SOLVE

Parameter	Type	Default	Description
ITMAX	integer	100	maximum # of Newton iterations
DELMAX	real	1×10^{-6}	convergence test (kT)
MAXDEL	real	1×10^{50}	
NDVRGE	integer	5	# of iterations for which ΔV can increase before divergence is assumed
NBACKUP	integer	3	
NDVBIG	integer	2	
METHOD	integer	1	
TAU	real	1.0	for METHOD=2

OUTPUT

Parameter	Type	Default	Description
INFO	integer	3	level of output 0 for mimimum 5 for debugging
STEP	integer	5	for tables, print values every STEP nodes
COPIES	integer	2	# copies of summary info

MESH

Parameter	Type	Default	Description
NX	integer	250	total # of nodes in F-D mesh
XRES	real	0.5	min. spatial resolution (angstroms)
MFLAG	integer	0	if =0, initial mesh is redefined based on refinement criteria described below if =1, mesh is not redefined
WT	real( )	 1.0 1.0 0.5 0.5	weighting parameters for mesh refinement WT(1), ρ slowly varying WT(2), **E** slowly varying WT(3), tendency for uniform mesh WT(4), tendency fo same # nodes in each LAYER
ISMTH0	integer	0	# of nodes set aside (per LAYER) for smoothing of redefined mesh
ISMTH1	integer	6	# of nodes set aside (per LAYER) for smoothing of initial mesh
XFIX	real( )	-1.	position(s) at which a node must be placed (angstroms) to enable, set XFIX(1)=0.0
NNX	integer( )	-1	# nodes to be placed between fixed node positions (positioning of these nodes is still based on redefinement scheme)

MISC

Parameter	Type	Default	Description
TEMPC	real	27.0	temperature (°C)
TEMPK	real	300.15	temperature (Kelvin)
VTH(300)	real	1×10^{7}	thermal velocity at 300 K (cm/s)

BC

Parameter	Type	Default	Description
MBC	integer	1	sets contact boundary conditions =1 for charge neutral contacts =2, then electrostatic potential at contacts set by metal work functions and semiconductor electron affinity, ϕ_{ms} =3 for front neutral, back ϕ_{ms} =4 for back neutral, front ϕ_{ms}
WDFRT	real	0.86	$\phi_M - \chi_S$ at front contact (eV)
WDBCK	real	0.86	$\phi_M - \chi_S$ at back contact (eV)
SPF	real	-1.0	surface recombination velocity for holes at x=0 (cm/s) (=–1 sets SPF=∞)
SNF	real	-1.0	surface recombination velocity for electrons at x=0 (cm/s)
SPB	real	-1.0	surface recombination velocity for holes at $x=x_{max}$ (cm/s)
SNB	real	-1.0	surface recombination velocity for electrons at $x=x_{max}$ (cm/s)

GLOBAL

This card must appear before any LAYER card. The default value for each variable on the LAYER card can be changed on this card (except T, the layer thickness).

*LAYER

All characters following *LAYER (up to column 75) become part of a comment used to annotate the output. It is intended to provide additional descriptive information about the associated LAYER.

LAYER

Parameter	Type	Default	Description
T	real		thickness of layer (angstroms)
TM	real		thickness of layer (microns)
EG EGL EGR	real	1.0	bandgap (eV)
CHI CHIL CHIR	real	4.0	electron affinity (eV)
KS	real	1.0	dielectric constant
NDX	real	1.0	index of refraction
NV NVL NVR	real	1×10^{20}	valence band effective density of states (cm^{-3})
NC NCL NCR	real	1×10^{20}	conduction band effective density of states (cm^{-3})
UP UPL UPR	real	1.0	hole mobility ($cm^2/V-s$)
VSATP	real		saturation vel. for holes (cm/sec)
BBP	real	2.0	power law for field dep mobility
UN UNL UNR	real	1.0	electron mobility ($cm^2/V-s$)
VSATN	real		saturation vel. for electrons (cm/sec)
BBN	real	2.0	power law for field dep mobility

LAYER (continued)

Parameter	Type	Default	Description
PROF.NA	char	LINEAR	doping profile type (only option at present)
NA NAL NAR	real real real	0.0	acceptor dopant density (cm^{-3})
NA.SIG	real	0.0	standard deviation (in eV) of gaussian distribution of acceptors
GA	real	1.0	acceptor degeneracy factor
EAA EAAL EAAR	real	0.0	acceptor energy level (eV above E_V)
XNA	real	0.0	(see notes) (angstroms)
PROF.ND	char	LINEAR	doping profile type (only option at present)
ND NDL NDR	real real real	0.0	donor dopant density (cm^{-3})
ND.SIG	real	0.0	standard deviation (in eV) of gaussian distribution of donors
GD	real	1.0	donor degeneracy factor
EAD EADL EADR	real	0.0	donor energy level (eV below E_C)
XND	real	0.0	(see notes) (angstroms)

LAYER (continued)

Parameter	Type	Default	Description
KTA.T	real	.001	characteristic energy of conduction band tail (eV)
KTD.T	real	.001	characteristic energy of valence band tail (eV)
GAMAX.T	real	0.0	density of states of conduction band tail at E_C (cm^{-3}–eV^{-1}) (-1. sets GAMAX.T = NC/(1eV)) (states assumed to be acceptor-like)
GDMAX.T	real	0.0	density of states of valence band tail at E_V (cm^{-3}–eV^{-1}) (-1. sets GDMAX.T = NV/(1eV)) (states assumed to be donor-like)
EACORN.T	real	0.0	energy below E_C at which conduction band tail begins (eV)
EDCORN.T	real	0.0	energy above E_V at which valence band tail begins (eV)
CAP.T	real	1×10^{-14}	capture cross-section for holes in the conduction band tail (cm^2)
CAN.T	real	1×10^{-14}	capture cross-section for electrons in the conduction band tail (cm^2)
CDP.T	real	1×10^{-14}	capture cross-section for holes in the valence band tail (cm^2)
CDN.T	real	1×10^{-14}	capture cross-section for electrons in the valence band tail (cm^2)

LAYER (continued)

Parameter	Type	Default	Description
A0	real	0	radiative recombination coeff. (cm^3/s)
AP	real	0	hole Auger coeff. (cm^6/s)
AN	real	0	electron Auger coeff. (cm^6/s)
TAUP.SHR	real(5)	1×10^6	SHR hole lifetime (s)
TAUN.SHR	real(5)	1×10^6	SHR electron lifetime (s)
ET.SHR	real(5)	0.0	SHR trap level wrt E_i (eV)
NTT.SHR	real(5)	0.0	density of SHR recomb centers (cm^{-3}) (donor-like, if NTT.SHR > 0) (acceptor-like, if NTT.SHR < 0)
SIG.SHR	real(5)	0.0	standard deviation (in eV) of gaussian SHR distribution
NTT.D	real	0.0	D level density (cm^{-3})
SIG.D	real	0.0	standard deviation (in eV) of gaussian D level distribution
ET.D+ ETL.D+ ETR.D+	real	0.5	D^+ trap level wrt E_V (eV)
ET.D- ETL.D- ETR.D-	real	0.5	D^- trap level wrt E_V (eV)
CP.D-	real	1×10^{-14}	$D^-\rightarrow D^0$ hole capture cross section (cm^2)
CP.D0	real	1×10^{-14}	$D^0\rightarrow D^+$ hole capture cross section (cm^2)
CN.D+	real	1×10^{-14}	$D^+\rightarrow D^0$ electron capture cross section (cm^2)
CN.D0	real	1×10^{-14}	$D^0\rightarrow D^-$ electron capture cross section (cm^2)

LAYER (continued)

Parameter	Type	Default	Description
EG1.OPT	real	-1.	optical bandgap (eV)
EG1L.OPT			(-1 sets EG1.OPT = EG)
EG1R.OPT			
C0.EG1	real	0.0	parameters used in optical
C1.EG1	real	0.0	absorption calculation
C2.EG1	real	0.0	
C3.EG1	real	0.0	
C4.EG1	real	0.0	
C5.EG1	real	0.0	
C6.EG1	real	0.0	
C7.EG1	real	0.0	
EG2.OPT	real	0.	optical bandgap (eV)
EG2L.OPT			
EG2R.OPT			
C0.EG2	real	0.0	parameters used in optical
C1.EG2	real	0.0	absorption calculation
C2.EG2	real	0.0	
C3.EG2	real	0.0	
C4.EG2	real	0.0	
C5.EG2	real	0.0	
C6.EG2	real	0.0	
C7.EG2	real	0.0	
EG3.OPT	real	0.0	optical bandgap (eV)
EG3L.OPT			
EG3R.OPT			
C0.EG3	real	0.0	parameters used in optical
C1.EG3	real	0.0	absorption calculation
C2.EG3	real	0.0	
C3.EG3	real	0.0	
C4.EG3	real	0.0	
C5.EG3	real	0.0	
C6.EG3	real	0.0	
C7.EG3	real	0.0	

LAYER (continued)

Parameter	Type	Default	Description
TAIL.OPT	logical	FALSE	if TRUE, absorption tail included
ALFC.OPT	real	0.0	parameters used in absorption
ZETA.OPT	real	0.0	tail calculation (see notes)
PH.OPT	logical	FALSE	if TRUE, phonon assisted absorption included
EP1.OPT	real	0.0	phonon assisted absorption
EP2.OPT	real	0.0	parameters (see notes)
ALF.OPT	real(6)		
MODEL	char		set parameters for specific materials =CIS.Cu- for Cu-poor CIS =CIS.Cu+ for Cu-rich CIS =CIS.st for Stoichometric CIS =i-CdS for intrinsic CdS =p-CdTe for p-type CdTe =n-CdTe for n-type CdTe =a-Si for α-Si

GENREC

Parameter	Type	Default	Description
GEN	char	DARK	sets generation rate options- DARK UNIFORM MONO (monochromatic) AM1P5G, etc. (see notes)
WL	real		wavelength for GEN=MONO (μm)
JINC	real	0.1	incident flux ×q (A/cm^2) (GEN=MONO,UNIFORM, or spectral response (SR) option)
CONC	real	1.0	multiplication factor for illumination intensity
SHADOW	real	0.0	relative shadowing factor
ANGLE	real	0.0	angle of incidence
RBACK	real	0.0	relative back surface reflectance
RFRONT	real	0.0	relative internal front surface reflectance

I-V

Parameter	Type	Default	Description
VSTART	real	0.0	start voltage (V)
VSTOP	real	0.0	stop voltage (V)
DV	real	0.0	voltage increment (V)
V	real( )	0.0	voltage (V)

SOLCELL

Parameter	Type	Default	Description
GFACTOR	integer	10	$10^{-GFACTOR}$ is the initial gereration rate factor for stepping up the intensity
VSTART	real	0.0	start voltage (V)
DVSMALL	real	0.03	smallest voltage increment (V)
DVBIG	real	0.10	largest voltage increment (V)
VSMALL	real	100.	voltage at which DVBIG becomes DVSMALL
RSERIES	real	0.0	external series resistance (Ω–cm^2)
RSHUNT	real	1×10^{51}	external shunt resistance (Ω–cm^2)

SR

Parameter	Type	Default	Description
VA	real	0.0	applied voltage (V)
J(VA)	real	0.0	dark current at V=VA (A/cm^2) (JA(VA) > 0 if VA > 0)
WL	real( )		wavelength (μm) defaults to WL=.34/.36/.38/.40/.44 /.46/.48/.50/.52/.54/.56/.58/.60 /.62/.64/.66/.68/.72/.76

IR

Parameter	Type	Default	Description
JINC	real	0.1	incident flux ×q (A/cm^2)
VA	real	0.0	applied voltage (V)
XMIN	real	0.0	start position for impulse response (μm)
XMAX	real	-1.0	stop position for impulse response (μm) (defaults to device length)
DX	real	-1.0	step size for impulse generation (μm) (defaults to 50 steps)

NOTES

Absorption Model

The absorption coefficient, $\alpha(E)$, is given by

$$\alpha = \alpha_1 + \alpha_2 + \alpha_3$$

with

$$\alpha_i = C0.EGi\, u(\Delta E) + C1.EGi\, \Delta E^{1/2} + \frac{C2.EGi}{E}\, \Delta E^{1/2} + C3.EGi\, \Delta E^{3/2}$$

$$+ \frac{C4.EGi}{E}\, \Delta E^{3/2} + \frac{C5.EGi}{E}\, \Delta E^{2} + C6.EGi\, E\, \Delta E^{2} + \frac{C7.EGi}{E}\, \Delta E^{3}$$

where E is the photon energy in Ev, $\Delta E = E - EGi.OPT$, u(E) is the step function, EGi.OPT is the optical bandgap as defined on the LAYER card, and Cj.EGi are coefficients such that α is in cm^{-1}.

PLOTA USERS GUIDE

Plots of the internal parameters simulated by ADEPT/F can be plotted in a TEKTOOL window on a SUN4 workstation by invoking the command:

/home/aquarium7/grayj/ADEPTF/STUFF/plota4

or on a SUN3 workstation by invoking the command:

/home/aquarium7/grayj/ADEPTF/STUFF/plota3

PLOTA is an interactive program which prompts the user for the required information. If requested, files which can be used to get hard copies of desired plots can be created. These files all have a '.plt' suffix.

These can be printed on an Apple laserwriter by using the batch file listed below:

/home/aquarium7/grayj/ADEPTF/lwplot:

```
(
cat /dev/null > temp.$$
for i
do
plot -Tpic $i | sed -e '1s/5/7/' | (echo '.bp';echo '.sp1i';cat - ) >> temp.$$
done
nmt -Tpsc -p - temp.$$ |lpr -PX -n
rm temp.$$
) &
```

where **X** identifies the desired laserwriter.

Or, these can be printed on an Imagen laserprinter by using the batch file listed below:

/home/aquarium7/grayj/ADEPTF/implot:

```
(
cat /dev/null > temp.$$
for i
do
plot -Tpic $i | sed -e '1s/5/7/' | (echo '.bp';echo '.sp1i';cat - ) >> temp.$$
done
nmt -Ti300 -p - temp.$$ |lpr -PX -n
rm temp.$$
) &
```

where **X** identifies the desired laserprinter.

Also, tables of the plot data can be requested which can then be imported into a spreadsheet program, plotting program, etc. These files all have a '.tbl' suffix.

AVAILABLE PLOTS

Plot	Description
excess	excess carrier concentration
logxcess	log of excess carrier concentration
carrier	carrier concentration
logcar	log of carrier concentration
potent	electrostatic potential
delpot	change from equilibrium of the electrostatic potential
dember	dember potential difference
resist	resistive potential difference
recrate	recombination rate
recomb1	recombination rate (tail & d-level components)
recomb2	recombination rate (b-b and Auger components)
current	current density
efield1	electric field
efield2	electric field
rho	total charge density
rho+rhog	total and gap charge densities
rhotd	tail and dangling bond charge densities
logrhotd	log of the above
rhogap	gap charge density
doping	doping density
eband	energy band diagram
genrate	generation rate
loggen	log of generation rate
mshspace	mesh
mshspac1	mesh
mshspac2	mesh
alpha	absorption coeff vs energy
sc	current-voltage for solar cell
iv	current-voltage
sr	spectral response
ir	impulse response
d-states	d-states vs. energy at xmin, xmax is min. density
t-states	t-states vs. energy at xmin, xmax is min. density