APPENDIX A

Fortran Variables in FG/DVC Submodel

FORTRAN VARIABLES IN FG/DVC SUBMODEL

Variable	Routine	Definition
a(i)	getkin	pre-exponential factors for fg reactions
aa	getkin	Arrhenius pre-exponential factor for reaction of abstracted part in secondary reactions submodel
aa1	reinit	mean value of the distribution function
aa2	reinit	standard deviation of the distribution function
aaaa(j,i)	getkin	Not used
aac	getkin	pre-exponential for acetylene (secondary reactions)
aacaac(j,i)	getkin	Not used
am	getkin	pre-exponential for missing (secondary reactions)
amam(j,k)	getkin	Not used
amonw(i)	polybd	mol. wt. of monomer i (real)
amvsol	datin	molar volume of pyridine (not used)
amwcol	datin	mol. wt. between crosslinks (not used)
aol	getkin	pre-exponential for olefins (secondary reactions)
aolaol(j,i)	getkin	Not used?
asoot	getkin	pre-exponential for soot (secondary reactions)
asz(1)	getkin	pre-exponential for sulfur? (secondary reactions); not used
asz(2)	getkin	pre-exponential for sulfur? (secondary reactions); not used
ax(2)	getkin	pre-exponential for tar (secondary reactions)
b(i)	getkin	activation energies for fg reactions

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
b(i)	getkin	activation energy for functional group i
ba	getkin	Activation energy for abstracted
bac	getkin	activation energy for acetylent (secondary reactions)
bead	datin	initial # of monomers
bm	getkin	activation energy for missing (secondary reactions)
bol	getkin	activation energy for olefins (secondary reactions)
bond(irow,icol)	bondw	bond type at icolth bond site on the irowth bead: 1–labile bond, 2–capped with CH_3, 3–hard bond, 4–capped with H (available for crosslinking), 5–capped with crosslink
bsoot	getkin	activation energy for soot (secondary reactions)
bsz(1)	getkin	activation energy for sulfur? (secondary reactions)
bsz(2)	getkin	activation energy for sulfur? (secondary reactions)
bx(2)	getkin	activation energy for tar (secondary reactions)
ca	getcdf	not used
cb	getcdf	not used
chem1(i)	polybd	monomer type for bead i
chem2(i)	polybd	oligomer # for bead i
chrate	heat	rate of char evolution, sec^{-1}
cnst2	datin	average pressure difference between the surface and the particle's interior
conc(1)	polybd	# ethylene bridges in char
conc(2)	polybd	# methyl groups in char

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
conc(3)	polybd	# hard bonds in char
conc(4)	rxn2	# bond sites currently capped with H and therefore available for crosslinking in char
conc(5)	rxn2	total # crosslinks in char
cs	getkin	not used
cumgas	dvc	total gas evolved
cvel	vpset0	constant used in the calculation of diffusivity of tar in the surrounding gas as a function of temperature and pressure
deltfg	psict	time interval for calling fgdvc submodel
deltim	monte	time increment for Monte Carlo calculations in DVC model
densty	datin	density of coal particle (g/cm^3)
dmass	polybd	mass of extractables
dphi	polybd	initial fraction of extractables
dqr	dvc	same as dsr
dsr	ther15	rate of total gas evolution for a time step
dst0(k,i)	reinit	density function for the k^{th} pool, i^{th} functional group
dvg1, dvg2,dvg3,dvg4	datin	constants in viscosity model
fethyl	datin	initial # hard bonds
fgdvc	pcgc2	if true, fgdvc submodel is used for coal devolatilization
flink	datin	initial # of crosslinks
gas	ther15	total gas evolution for a time step
gd	datin	temp. where heating rate changes (not used)

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
gd2	datin	second heating rate (not used)
heatrt	psict	
hoxid	heat	heat of combustion of coal (used as heat of oxidation of char), J/kg, not used
k1	dvc	bond-breaking rate calculated by FG and sent to DVC (same as tarfac)
kays(i)	tblrts	reaction rate coefficients for fg reactions
lcdvc	psict	if true, dvc calculations are performed
lpyrol	psict	true if particle is undergoing pyrolysis
mass	dvc	total mass of coal sample
mass0	polybd	initial mass of sample coal
masslm(1)	datin	lower molecular weight limit of first char bin
masslm(2)	datin	width of char bins
maxk	pools.inc	no. of points for integration over distributed activation energy
mermas(i)	datin	masses of char bins
mermax	dvccom.inc	max. # char bins
mers	datin	# of char bins for vaporization
mmass(i)	datin	mol. wt. of monomer i (integer)
mnumb(i)	datin	% of each monomer type (integer)
mono	datin	# of monomer types
mrange	dvccom.inc	mass range for mass spectra
ms(jmass)	monte	# of oligomers of molecular weight jmass that have vaporized as tar
msfr	monte	ratio of initial coal sample mass used for DVC simulation to total initial coal particle mass

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
nbead(i)	polybd	# beads of each monomer type
nbpo	polybd	# beads per oligomer at the beginning
ncmax	dvccom.inc	max. # different bond types
ncoal2	coal2	No. of calls to coal2 subroutine for a given trajectory
nfgout	psict	
nomax	dvccom.inc	max # of oligomers in sample
numbnd	rxn1	keeps track of number of broken bonds during each call to DVC
oligo	inipol	# of oligomers
oligst	datin	initial # of oligomers
olims	polybd,dvc	# of oligomers with mass greater than zero
omass(i)	polybd	mass of each oligomer
omers(i)	olimer	# oligomers in i^{th} char bin
point(i)	rxn2	points to bead # of bead that i^{th} bead is cross-linked or bonded to (if any)
press	datin	ambient pressure
rad	vapvel	particle radius
radi0	psict	initial particle radius
rhpyro	heat	rate of released heat of pyrolysis, J sec^{-1} kg^{-1}
rtcont(k)	ther15	rate constant of each functional group, sec^{-1}
rvle	heat	rate of volatiles enthalpy, J sec^{-1} kg^{-1}
sigmaa(i)	getkin	variance of activation energy for functional group i
tarfac	ther15	bond-breaking rate calculated by FG and sent to DVC

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
tarmas	monte	total mass of tar evaporated from the coal sample on a call to dvc
tarrat	psict	
tclock	ther15	time at which the next call to the FG/DVC submodel will be made
tconc(i)	olivap	same as conc(i) except it's for the ta:
temp		particle temperature
timdel	ther15	time interval until the next call to FG/DVC will be made
timdel	dvc	time step in FG/DVC submodel
time	ther15	time step in FG model
time	psict	total particle trajectory time
time	dvc	
timefg	psict	time at which next call to FGDVC should take place
timmx	dvc	
timsum	ther15	total time for each call to FG/DVC
tmass0	polybd	total initial mass of the coal sample (same as mass0, except real number)
totcha	dvc	same as mass except normalized to mass0
tottar	dvc	same as ytar except accumulated for the whole trajectory
vap0	vpset0	constant used for calculating the coal sample radius which is assumed to shrink with the cubic root of its mass
vap1	vpset0	constant used for calculating the coal sample volume
viseng	datin	constant in viscosity model
vsrcol	datin	swelling ratio of raw coal (not used)

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
vsrmin	datin	minimum swelling ratio of char (not used)
vstmax	datin	constant in viscosity model
vvel(i)	vapvel	
vvel0(i)	vapset	
vvel2(i)	vpset0	constant used in the calculation of external transport of tars from the particle surface to the bulk gas using the model of Unger and Suuberg
vvel3(i)	vpset0	constant used in the correlation of Unger and Suuberg for calculating vapor pressure of high molecular weight aromatics with aliphatic side-chains
wa(i)		
wac(i)	ther15	
wacs(j,i)		
wc(1,i),wc(2,i)	reinit	same as wc0(1,i),wc0(2,i) except this is the current value, based on the original coal sample
wc(2,i)	ther15	composition of char
wc0(1,i)	inity0	initial composition of functional group i (non-tar forming); not used in combined FG/DVC model
wc0(2,i)	inity0	initial composition of functional group i(potentially tar-forming)
wchld(i)		
wcs(i)	ther15	rate constant (beginning of ther15); evolution of pool i in a time step (latter portion of ther15)
wct(i)	ther15	same as wc(2,i)
wctfg(i)	finfl1	mass fraction of each functional group
wctot		

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
wg(i)	ther15	same as wgs(2,i)
wghld(i)		
wgs(1,i)	ther15	not used in combined FG/DVC model
wgs(2,i)	ther15	weight fraction in the evolved gas
wgtot		
wm(i)	finfl1	
wmhld(i)		
wol(i)		
wols(j,i)		
wsoot(i)		
wsoots(j,i)		
wt(i)	ther15	same as wts(2,i)
wthld(i)		
wts(1,i)	ther15	not used in combined FG/DVC model
wts(2,i)	ther15	weight fraction in the tar
wttot		
x02	getcdf	wt. frac. of coal that is potentially tar-forming
xco0	getcdf	weight percent carbon in original daf coal
xeff(i)	datin	cross-linking efficiency
xho0	getcdf	wt. % hydrogen in original daf coal
xlink	ther15	# of cross-links to form per gram of coal due to gas evolution
xno0	getcdf	wt. % nitrogen in original daf coal
xo0	getcdf	wt. % oxygen in original daf coal
xoh	getcdf	wt. frac. of coal that is OH groups

FORTRAN VARIABLES IN FG/DVC SUBMODEL (continued)

Variable	Routine	Definition
xoxid	coal2	total oxidation rate on per unit mass basis, sec^{-1}
xsm0	getcdf	not used
xso0	getcdf	wt. % sulfur in original daf coal
xt0	datin	starting extractables, experimental (not used)
xtar	ther15	total tar until that time step; position "x" in FG
xxx	inity0, finfl1	mole ratio of aliphatic hydrogen to aliphatic carbon (not used)
y0(i)	getcdf	wt. frac. of coal that is functional group i
y0tot	inity0	sum of y0's for functional group pools 1 through 27
y0tots	inity0	sum of y0's for functional group pools 1 through 30
ylink	dvc	cumulative xlinks
ytar	dvc	same as tarmas except normalized to initial mass of coal sample

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