

INPUT FILES

Type	File name	Description	Requirement
problem specific input files	prefix.dat	General problem specific input	Required
	prefix.tem	Depth dependent temperature field	Optional
	prefix.ivs	Initial condition for flow simulation	Optional
database files	comp.dbs	Components	Required
	complex.dbs	Aqueous complexation	Required
	redox.dbs	Oxidation-reduction	Required
	gases.dbs	Gas dissolution-exsolution	Required
	sorption.dbs	Ion exchange	Required
	mineral.dbs	Mineral dissolution-precipitation	Required

OUTPUT FILES

General Model output and flow solution

File name	Description	TECPLOT Header
prefix_o.gen	General problem specific output, contains feed-back from input file and results of batch simulations including the equilibration of background and source water chemistry Output format: assorted Suffix meaning: gen = general	N
prefix.log	run-specific information on convergence and trouble shooting Output format: assorted Suffix meaning: log = logbook	N
prefix_x.gsp	hydraulic head, pressure head, water and gas saturations, moisture and gas contents at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsp = global/spatial/pressure	Y
prefix_x.vel	interfacial velocities at output time x (0 = initial condition) – contour data Output format: x,(y),(z), v_x , (v_y), (v_z) Suffix meaning: vel = velocities	Y

Reactive transport solution – contour data

File name	Description	TECPLOT Header
prefix_x.gst	total aqueous component concentrations at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gst = global/spatial/total aqueous component concentrations	Y
prefix_x.gsc	aqueous species concentrations at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsc = global/spatial/species concentrations	Y
prefix_x.gsi	reaction rates of intra-aqueous kinetic reactions at output time x – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsi = global/spatial/intra-aqueous kinetic reactions	Y
prefix_x.gsm	master variables (pH, pe, Eh, ionic strength, alkalinity, temperature) at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsm = global/spatial/master variables	Y

prefix_x.gsg	partial gas pressures at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsg = global/spatial/partial gas pressures	Y
prefix_x.gsgr	degassing rates at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsgr – global/spatial/degassing/rates	Y
prefix_x.gsv	mineral volume fractions at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsv – global/spatial/volume fractions	Y
prefix_x.gsb	surface species at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsb – global/spatial/sorbed species	Y
prefix_x.gss	mineral saturation indices at output time x (0 = initial condition) – contour data Output format: x,(y),(z), parameter values Suffix meaning: gss – global/spatial/saturation indices	Y

Reactive Transport – transient data

File name	Description	TECPLOT Header
prefix_x.gsd	mineral dissolution-precipitation rates at output time x – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsd = global/spatial/dissolution- precipitation rates	Y
prefix_x.gsx	saturation indices of excluded minerals at output time x – contour data Output format: x,(y),(z), parameter values Suffix meaning: gsd = global/spatial/excluded minerals	Y
prefix_x.gbt	total aqueous component concentrations at output location x – transient data Output format: time, parameter values Suffix meaning: gbt = global/breakthrough/total aqueous component concentrations	Y
prefix_x.gbc	aqueous species concentrations at output location x – transient data Output format: time, parameter values Suffix meaning: gbc = global/breakthrough/species concentrations	Y

prefix_x.gbi	reaction rates of intra-aqueous kinetic reactions at output location x – transient data Output format: time, parameter values Suffix meaning: gbi = global/breakthrough/intra-aqueous kinetic reactions	Y
prefix_x.gbm	master variables (pH, pe, Eh, ionic strength, alkalinity, temperature) at output location x – transient data Output format: time, parameter values Suffix meaning: gbm = global/breakthrough/master variables	Y
prefix_x.gbg	partial gas pressures at output location x – transient data Output format: time, parameter values Suffix meaning: gbg = global/breakthrough/partial gas pressures	Y
prefix_x.gbgr	degassing rates at output location x – transient data Output format: time, parameter values Suffix meaning: gbgr – global/breakthrough/degassing/rates	Y
prefix_x.gbv	mineral volume fractions at output location x – transient data Output format: time, parameter values Suffix meaning: gbv – global/breakthrough/volume fractions	Y
prefix_x.gbb	surface species at output location x – transient data Output format: time, parameter values Suffix meaning: gbb – global/breakthrough/sorbed species	Y
prefix_x.gbs	mineral saturation indices at output location x – transient data Output format: time, parameter values Suffix meaning: gbs – global/breakthrough/saturation indices	Y
prefix_x.gbd	mineral dissolution-precipitation rates at output location x – transient data Output format: time, parameter values Suffix meaning: gbd = global/breakthrough/dissolution-precipitation rates	Y
prefix_x.gbx	saturation indices of excluded minerals at output location x – transient data Output format: time, parameter values Suffix meaning: gbx = global/breakthrough/excluded minerals	Y

Output, Local Geochemistry

prefix_x.lbt	total aqueous component, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbt = local/breakthrough/total aqueous component concentrations	Y
prefix_x.lbc	aqueous species concentrations, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbc = local/breakthrough/species concentrations	Y
prefix_x.lbi	reaction rates of intra-aqueous kinetic reactions, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbi = local/breakthrough/intra-aqueous kinetic reactions	Y
prefix_x.lbm	master variables (pH, pe, Eh, ionic strength, alkalinity, temperature) , local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbm = local/breakthrough/master variables	Y
prefix_x.lbg	partial gas pressures, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbg = local/breakthrough/partial gas pressures	Y
prefix_x.lbgr	degassing rates, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbgr – local/breakthrough/degassing/rates	Y
prefix_x.lbv	mineral volume fractions, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbv – local/breakthrough/volume fractions	Y
prefix_x.lbb	surface species, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbb – local/breakthrough/sorbed species	Y
prefix_x.lbs	mineral saturation indices, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbs – local/breakthrough/saturation indices	Y
prefix_x.lbd	mineral dissolution-precipitation rates, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbd = local/breakthrough/dissolution-precipitation rates	Y

prefix_x.lbx	saturation indices of excluded minerals, local geochemistry – transient data, or pC-pH-data Output format: time or pH, parameter values Suffix meaning: lbx = local/breakthrough/excluded minerals	Y
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