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** = **gen**eral	N
`prefix.log`	run-specific information on convergence and trouble shooting Output format: assorted Suffix meaning: **log** = **log**book	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** = **g**lobal/**s**patial/**p**ressure	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** = **vel**ocities	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** = **g**lobal/**s**patial/**t**otal 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** = **g**lobal/**s**patial/**s**pecies 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** = **g**lobal/**s**patial/**i**ntra-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** = **g**lobal/**s**patial/**m**aster variables	Y

File name	Description	TECPLOT Header
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** = **g**lobal/**s**patial/**p**artial **g**as 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** – **g**lobal/**s**patial/**d**e**g**assing/**r**ates	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** – **g**lobal/**s**patial/**v**olume 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** – **g**lobal/**s**patial/sor**b**ed 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** – **g**lobal/**s**patial/**s**aturation 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** = **g**lobal/**s**patial/**d**issolution-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** = **g**lobal/**s**patial/e**x**cluded minerals	Y
prefix_x.gbt	total aqueous component concentrations at output location x – transient data Output format: time, parameter values Suffix meaning: **gbt** = **g**lobal/**b**reakthrough/**t**otal aqueous component concentrations	Y
prefix_x.gbc	aqueous species concentrations at output location x – transient data Output format: time, parameter values Suffix meaning: **gbc** = **g**lobal/**b**reakthrough/species **c**oncentrations	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** = **g**lobal/**b**reakthrough/**i**ntra-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** = **g**lobal/**b**reakthrough/**m**aster variables	Y
prefix_x.gbg	partial gas pressures at output location x – transient data Output format: time, parameter values Suffix meaning: **gbg** = **g**lobal/**b**reakthrough/partial **g**as pressures	Y
prefix_x.gbgr	degassing rates at output location x – transient data Output format: time, parameter values Suffix meaning: **gbgr** – **g**lobal/**b**reakthrough/degassing/**r**ates	Y
prefix_x.gbv	mineral volume fractions at output location x – transient data Output format: time, parameter values Suffix meaning: **gbv** – **g**lobal/**b**reakthrough/**v**olume fractions	Y
prefix_x.gbb	surface species at output location x – transient data Output format: time, parameter values Suffix meaning: **gbb** – **g**lobal/**b**reakthrough/sor**b**ed species	Y
prefix_x.gbs	mineral saturation indices at output location x – transient data Output format: time, parameter values Suffix meaning: **gbs** – **g**lobal/**b**reakthrough/**s**aturation indices	Y
prefix_x.gbd	mineral dissolution-precipitation rates at output location x – transient data Output format: time, parameter values Suffix meaning: **gbd** = **g**lobal/**b**reakthrough/**d**issolution-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** = **g**lobal/**b**reakthrough/e**x**cluded 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** = **l**ocal/**b**reakthrough/**t**otal 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** = **l**ocal/**b**reakthrough/species **c**oncentrations	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** = **l**ocal/**b**reakthrough/**i**ntra-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** = **l**ocal/**b**reakthrough/**m**aster 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** = **l**ocal/**b**reakthrough/partial **g**as 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** – **l**ocal/**b**reakthrough/degassing/**r**ates	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** – **l**ocal/**b**reakthrough/**v**olume 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** – **l**ocal/**b**reakthrough/sor**b**ed 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** – **l**ocal/**b**reakthrough/**s**aturation 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** = **l**ocal/**b**reakthrough/**d**issolution-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/**b**reakthrough/e**x**cluded minerals	Y