**Test.dat**

Components: CO3, H

Species:

[OH] = [H]-1\*Kw

[HCO3] = [H] \* [CO3] \* KHCO3

[H2CO3] = [H]2\*[CO3]\*KH2CO3

Totals:

T.CO3 = [CO3] + [HCO3] + [H2CO3]

T.H = [H] – [OH] + [HCO3] + 2\*[H2CO3]

Residuals:

R.CO3 = [CO3] + [H] \* [CO3] \* KHCO3+ [H]2\*[CO3]\*KH2CO3 – T.CO3known

R.H = [H] – [H]-1\*Kw + [H] \* [CO3] \* KHCO3+ 2\*[H]2\*[CO3]\*KH2CO3 – T.Hknown

Derivatives:

Jacobian:

**Abbrev\_inorg.dat**

Components: Cu, CO3, H

Species:

[OH] = [H]-1\*Kw

[HCO3] = [H] \* [CO3] \* KHCO3

[H2CO3] = [H]2\*[CO3]\*KH2CO3

[CuHCO3] = [Cu]\*[H]\*[CO3]\*KCuHCO3

Totals:

T.Cu = [Cu] + [CuHCO3]

T.CO3 = [CO3] + [HCO3] + [H2CO3]

T.H = [H] – [OH] + [HCO3] + 2\*[H2CO3]

Residuals:

R.Cu = [Cu] + [Cu][H][CO3]KCuHCO3 – T.Cuknown

R.CO3 = [CO3] + [H][CO3]KHCO3 + [H]2[CO3]KH2CO3 + [Cu][H][CO3]KCuHCO3 – T.CO3known

R.H = [H] – [H]-1Kw + [H][CO3]KHCO3+ 2[H]2[CO3]KH2CO3+[Cu][H][CO3]KCuHCO3 – T.Hknown

Derivatives:

Jacobian:

**Abbrev\_inorg\_wBL.dat**

Components: Cu, CO3, BL, H

Species:

[OH] = [H]-1\*Kw

[HCO3] = [H] \* [CO3] \* KHCO3

[H2CO3] = [H]2\*[CO3]\*KH2CO3

[CuHCO3] = [Cu]\*[H]\*[CO3]\*KCuHCO3

[BL-Cu] = [BL]\*[Cu]\*KBL-Cu

[BL-H] = [BL]\*[H]\*KBL-H

Totals:

T.Cu = [Cu] + [CuHCO3]+[BL-Cu]\*CtoMBL

T.CO3 = [CO3] + [HCO3] + [H2CO3]

T.BL = ([BL] + [BL-Cu] + [BL-H])\*CtoMBL

T.H = [H] – [OH] + [HCO3] + 2\*[H2CO3]+[BL-H]\*CtoMBL

Residuals:

R.Cu = [Cu] + [Cu][H][CO3]KCuHCO3 + [BL][Cu]K­BL-Cu\*CtoMBL – T.Cuknown

R.CO3 = [CO3] + [H][CO3]KHCO3 + [H]2[CO3]KH2CO3 + [Cu][H][CO3]KCuHCO3 – T.CO3known

R.BL = ([BL] + [BL][Cu]KBL-Cu + [BL][H]KBL-H )\*CtoMBL– T.BLknown

R.H = [H] – [H]-1Kw + [H][CO3]KHCO3+ 2[H]2[CO3]KH2CO3+[Cu][H][CO3]KCuHCO3 + [BL][H]KBL-H\*CtoMBL – T.Hknown

Derivatives:

Jacobian:

**test\_wBL.dat**

Components: CO3, BL, H

Species:

[OH] = [H]-1\*Kw

[HCO3] = [H] \* [CO3] \* KHCO3

[H2CO3] = [H]2\*[CO3]\*KH2CO3

[BL-H] = [BL]\*[H]\*KBL-H

Totals:

T.CO3 = [CO3] + [HCO3] + [H2CO3]

T.BL = ([BL] + [BL-H])\*CtoMBL

T.H = [H] – [OH] + [HCO3] + 2\*[H2CO3]+[BL-H]\*CtoMBL

Residuals:

R.CO3 = [CO3] + [H][CO3]KHCO3 + [H]2[CO3]KH2CO3 – T.CO3known

R.BL = ([BL] + [BL][H]KBL-H )\*CtoMBL– T.BLknown

R.H = [H] – [H]-1Kw + [H][CO3]KHCO3+ 2[H]2[CO3]KH2CO3 + [BL][H]KBL-H\*CtoMBL – T.Hknown

Derivatives:

Jacobian:

**Filename: abbrev\_organic.dat4/.blm4**

Components: Cu, Na, Cl, H, DOC-FA, DL

Species:

[OH] = [H]-1\*Kw

[CuOH] = [Cu]\*[OH]\*KCuOH = [Cu]\* [H]-1\*Kw \*KCuOH

[CuCl] = [Cu]\*[Cl]\*KCuCl

[DOC] = [H-DOC]\*[H]-1\*KH-DOC

[Cu-DOC] = [Cu]\*[DOC]\*KCu-DOC = [Cu]\* [H-DOC]\*[H]-1\*KH-DOC\*KCu-DOC

[Na-DOC] = [Na]\*[DOC]\*KNa-DOC

[DL-H] = [H]\*DLFA \*KDL-H 🡪 🡪 [DL-H] <-> [H] + |zH|\* DLFA KDL-H = Ksel(H)=1

[DL-Cu] = [Cu] \* DLFA2 \*KDL-Cu 🡪 🡪 [DL-Cu] <-> [Cu] + |zCu|\* DLFA KDL-Cu = Ksel(Cu)=1

[DL-Na] = [Na] \* DLFA\*KDL-Na 🡪 🡪 [DL-Na] <-> [Na] + |zNa|\* DLFA KDL-Na = Ksel(Na) = 1

[DL-Cl] = [Cl] \* DLFA \*KDL-Cl 🡪 🡪 [DL-Cl] <-> [Cl] + |zCl|\* DLFA KDL-Cl = Ksel(Cl) = 1

[DL-OH] = [OH] \* DLFA = [H]-1 \* Kw \* DLFA\*KDL-OH 🡪 🡪 [DL-OH] <-> -1\*[H] + |zOH|\* DLFA KDL-OH = Ksel(OH)\*Kw

[DL-CuOH] = [CuOH] \* DLFA\*KDL-CuOH = [Cu]\* [H]-1\*Kw \*KCuOH \* DLFA\*KDL-CuOH 🡪 🡪 [DL-CuOH] <-> [Cu] - [H] + |zCuOH|\* DLFA KDL-CuOH = Ksel(CuOH) \*Kw \*KCuOH

[DL-CuCl] = [CuCl] \* DLFA\*KDL-CuCl = [Cu]\* [Cl]\*KCuCl \* RFA\*KDL-CuCl 🡪 🡪 [DL-CuCl] <-> [Cu] + [Cl] + |zCuCl|\* DLFA KDL-Cl = Ksel(CuCl) \*KCuCl

[DL-Cu(CO3)2] = [Cu(CO3)2]\*DLFA2\*KDL-Cu(CO3)2 = [Cu]\*[CO3]2\*DLFA2\*KCu(CO3)2\*KDL-Cu(CO3)2 🡪🡪   
 [DL-Cu(CO3)2] <-> [Cu] + 2\*[CO3] + 2\*[DLFA]

Totals:

T.Cu = [Cu] + [CuOH] + [CuCl] + [Cu-DOC] + [DL-Cu] + [DL-CuOH] + [DL-CuCl]

T.Na = [Na] + [Na-DOC] + [DL-Na]

T.Cl

T.BL = ([BL] + [BL-Cu] + [BL-H])\*CtoMBL

T.H = [H] – [OH] - [CuOH] - [DOC] – [Cu-DOC] – [Na-DOC] + [DL-H] – [DL-OH] – [DL-CuOH]

T.DLFA = 1\*[DL-H] + 2\*[DL-Cu] + 1\*[DL-Na] + 1\*[DL-CuOH] + 1\*[DL-Cl] - 1\*[DL-Cl] – 1\*[DL-OH]

T.DLFA = 1\*[H]\*DLFA\*KDL-H +2\*[Cu] \* DLFA2 \*KDL-Cu + 1\*[DL-Na] – 1\*[DL-Cl] – 1\*[DL-OH] – 1\*[Cu]\* [H]-1\*Kw \*KCuOH \* DLFA\*KDL-CuOH  - 1\*[DL-Cl]

Residuals:

R.Cu = [Cu] + [Cu]\* [H]-1\*Kw \*KCuOH + [Cu]\*[Cl]\*KCuCl + [Cu]\*[DOC]\*KCu-DOC + [Cu] \* DLFA2 \*KDL-Cu + [Cu]\* [H]-1\*Kw \*KCuOH \* DLFA +[Cu]\* [Cl]\*KCuCl \* DLFA – T.Cuknown

R.CO3 = [CO3] + [H][CO3]KHCO3 + [H]2[CO3]KH2CO3 + [Cu][H][CO3]KCuHCO3 – T.CO3known

R.BL = ([BL] + [BL][Cu]KBL-Cu + [BL][H]KBL-H )\*CtoMBL– T.BLknown

R.H = [H] – [H]-1Kw + [H][CO3]KHCO3+ 2[H]2[CO3]KH2CO3+[Cu][H][CO3]KCuHCO3 + [BL][H]KBL-H\*CtoMBL – T.Hknown

R.DL­FA = T.DLFA + ZFA = [H]\*DLFA\*KDL-H +2\*[Cu] \* DLFA2 \*KDL-Cu + [DL-Na] - [DL-Cl] - [DL-OH] - [DL-CuOH] - [DL-Cl] + ZFA

Derivatives:

Jacobian: