**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, DL, DOCwH, DOCsH

Species Reactions:

[Cu] = [Cu], K = 1, charge = +2

[Na] = [Na], K = 1, charge = +1

[Cl] = [Cl], K = 1, charge = -1

[H] = [H], K = 1, charge = +1

[DL] = ? , charge = 0

[DOCwH] = [DOCwH], K = 1, charge = 0

[DOCsH] = [DOCsH], K = 1, charge = 0

[OH] = -1\*[H], Kw = 10-13.997, charge = -1

[CuOH] = [Cu] + -1\*[H], KCuOH = 10-7.52, charge = +1

[CuCl] = [Cu] + [Cl], K = 100.4, charge = +1

[DL-Cu] = 2\*[DL] + [Cu], K = 1, charge = +2

[DL-Na] = [DL] + [Na], K = 1, charge = +1

[DL-Cl] = [DL] + [Cl], K = 1, charge = -1

[DL-H] = [DL] + [H], K = 1, charge = +1

[DL-OH] = [DL] + -1\*[H], K = 10-13.997, charge = -1

[DL-CuOH] = [DL] + [Cu] + -1\*[H], K=10-7.52, charge = +1

[DL-CuCl] = [DL] + [Cu] + [Cl], K = 100.4, charge = +1

[DOCw] = [DOCwH] + -1\*[H], K = 10-1.59, charge = -1

[DOCs] = [DOCsH] + -1\*[H], K = 10-12.4, charge = -1

[DOCw-Cu] = [DOCwH] + -1\*[H] + [Cu], K = 10-0.8, charge = +1

[DOCs-Cu] = [DOCsH] + -1\*[H] + [Cu], K = 10-3.168, charge = +1

[DOCw-CuOH] = [DOCwH] + -2\*[H] + [Cu], K = 10-8.32, charge = 0

[DOCs-CuOH] = [DOCsH] + -2\*[H] + [Cu], K = 10-10.688, charge = 0

Species Equations:

[Cu] = [Cu]

[Na] = [Na]

[Cl] = [Cl]

[H] = [H]

[DL] = ?

[DOCwH] = [DOCwH]

[DOCsH] = [DOCsH]

[OH] = [H]-1\*10-13.997

[CuOH] = [Cu]\*[H]-1\*10-7.52

[CuCl] = [Cu]\*[Cl]\*100.4

[DL-Cu] = [DL]2\*[Cu]

[DL-Na] = [DL]\*[Na]

[DL-Cl] = [DL]\*[Cl]

[DL-H] = [DL]\*[H]

[DL-OH] = [DL]\*[H]-1\*10-13.997

[DL-CuOH] = [DL]\*[Cu]\*[H]-1\*10-7.52

[DL-CuCl] = [DL]\*[Cu]\*[Cl]\*100.4

[DOCw] = [DOCwH]\*[H]-1\*10-1.59

[DOCs] = [DOCsH] \*[H]-1\*10-12.4

[DOCw-Cu] = [DOCwH]\*[H]-1\*[Cu]\*10-0.8

[DOCs-Cu] = [DOCsH]\*[H]-1 \*[Cu]\*10-3.168

[DOCw-CuOH] = [DOCwH]\*[H]-2\*[Cu]\*10-8.32

[DOCs-CuOH] = [DOCsH]\*[H]-2\*[Cu]\*10-10.688

Totals (in terms of species concentrations):

T.Cu = [Cu]\*Msol + [CuOH]\*Msol + [CuCl]\*Msol + [DL-Cu]\*MDL + [DL-CuOH]\*MDL + [DL-CuCl]\*MDL + [DOCw-Cu]\*Msol + [DOCs-Cu]\*Msol + [DOCw-CuOH]\*Msol + [DOCs-CuOH]\*Msol

T.Na = [Na]\*Msol + [DL-Na]\*MDL

T.Cl = [Cl]\*Msol + [CuCl]\*Msol + [DL-Cl]\*MDL + [DL-CuCl]\*MDL

T.H = [H]\*Msol + -1\*[OH]\*Msol + -1\*[CuOH] \*Msol + [DL-H]\*MDL + -1\*[DL-OH]\*MDL + -1\*[DL-CuOH]\*MDL + -1\*[DOCw]\*Msol + -1\*[DOCs]\*Msol + -1\*[DOCw-Cu]\*Msol + -1\*[DOCs-Cu]\*Msol + -2\*[DOCw-CuOH]\*Msol + -2\*[DOCs-CuOH]\*Msol

T.DL = 2\*[DL-Cu]\*MDL + [DL-Na]\*MDL + [DL-Cl]\*MDL + [DL-H]\*MDL + [DL-OH]\*MDL + [DL-CuOH]\*MDL + [DL-CuCl]\*MDL

T.DOCwH = [DOCwH]\*Msol + [DOCw]\*Msol + [DOCw-Cu]\*Msol + [DOCw-CuOH]\*Msol

T.DOCsH = [DOCsH]\*Msol + [DOCs]\*Msol + [DOCs-Cu]\*Msol + [DOCs-CuOH]\*Msol

Totals (in terms of component concentrations and K’s):

T.Cu = [Cu]\*Msol + [Cu]\*[H]-1\*10-7.52\*Msol + [Cu]\*[Cl]\*100.4\*Msol + [DL]2\*[Cu]\*MDL + [DL]\*[Cu]\*[H]-1\*10-7.52\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL + [DOCwH]\*[H]-1\*[Cu]\*10-0.8\*Msol + [DOCsH]\*[H]-1 \*[Cu]\*10-3.168\*Msol + [DOCwH]\*[H]-2\*[Cu]\*10-8.32\*Msol + [DOCsH]\*[H]-2\*[Cu]\*10-10.688\*Msol

T.Na = [Na]\*Msol + [DL]\*[Na]\*MDL

T.Cl = [Cl]\*Msol + [Cu]\*[Cl]\*100.4\*Msol + [DL]\*[Cl]\*MDL + [DL-CuCl]\*MDL

T.H = [H]\*Msol + -1\*[H]-1\*10-13.997\*Msol + -1\*[Cu]\*[H]-1\*10-7.52 \*Msol + [DL]\*[H]\*MDL + -1\*[DL]\*[H]-1\*10-13.997\*MDL + -1\*[DL]\*[Cu]\*[H]-1\*10-7.52\*MDL + -1\*[DOCwH]\*[H]-1\*10-1.59\*Msol + -1\*[DOCsH] \*[H]-1\*10-12.4\*Msol + -1\*[DOCwH]\*[H]-1\*[Cu]\*10-0.8\*Msol + -1\*[DOCsH]\*[H]-1 \*[Cu]\*10-3.168\*Msol + -2\*[DOCwH]\*[H]-2\*[Cu]\*10-8.32\*Msol + -2\*[DOCsH]\*[H]-2\*[Cu]\*10-10.688\*Msol

T.DL = 2\*[DL]2\*[Cu]\*MDL + [DL]\*[Na]\*MDL + [DL]\*[Cl]\*MDL + [DL]\*[H]\*MDL + [DL]\*[H]-1\*10-13.997\*MDL + [DL]\*[Cu]\*[H]-1\*10-7.52\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL

T.DOCwH = [DOCwH]\*Msol + [DOCwH]\*[H]-1\*10-1.59\*Msol + [DOCwH]\*[H]-1\*[Cu]\*10-0.8\*Msol + [DOCwH]\*[H]-2\*[Cu]\*10-8.32\*Msol

T.DOCsH = [DOCsH]\*Msol + [DOCsH] \*[H]-1\*10-12.4\*Msol + [DOCsH]\*[H]-1 \*[Cu]\*10-3.168\*Msol + [DOCsH]\*[H]-2\*[Cu]\*10-10.688\*Msol

Others:

Z = -1\*[DOCw] + -1\*[DOCs] + [DOCw-Cu] + [DOCs-Cu]

IS = 0.5\*([Cu]\*4 + [Na] + [Cl] + [H] + [OH] + [CuOH] + [CuCl] + [DL-Cu]\*4 + [DL-Na] + [DL-Cl] + [DL-H] + [DL-OH] + [DL-CuOH] + [DL-CuCl] + [DOCw] + [DOCs] + [DOCw-Cu] + [DOCs-Cu])

Residuals:

R.Cu = T.Cu– T.Cuknown

R.Na = T.Na – T.Na­known

R.Cl = T.Cl – T.Clknown

R.H = 0

R.DL = T.DL + Z

R.DOCwH = T.DOCwH – T.DOCwHknown

R.DOCsH = T.DOCsH – T.DOCsHknown

Residuals (in terms of components):

R.Cu = [Cu]\*Msol + [Cu]\*[H]-1\*10-7.52\*Msol + [Cu]\*[Cl]\*100.4\*Msol + [DL]2\*[Cu]\*MDL + [DL]\*[Cu]\*[H]-1\*10-7.52\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL + [DOCwH]\*[H]-1\*[Cu]\*10-0.8\*Msol + [DOCsH]\*[H]-1 \*[Cu]\*10-3.168\*Msol + [DOCwH]\*[H]-2\*[Cu]\*10-8.32\*Msol + [DOCsH]\*[H]-2\*[Cu]\*10-10.688\*Msol – T.Cuknown

R.Na = T.Na – T.Na­known

R.Cl = T.Cl – T.Clknown

R.H = 0

R.DL = 2\*[DL]2\*[Cu]\*MDL + [DL]\*[Na]\*MDL + [DL]\*[Cl]\*MDL + [DL]\*[H]\*MDL + [DL]\*[H]-1\*10-13.997\*MDL + [DL]\*[Cu]\*[H]-1\*10-7.52\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL + Z

R.DOCwH = T.DOCwH – T.DOCwHknown

R.DOCsH = T.DOCsH – T.DOCsHknown

Derivatives:

Jacobian: