**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: