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

Components: Cu, Na, Cl, H, DL, DOCwH, DOCsH

Species Reactions:

1. [Cu] = [Cu], K = 1, charge = +2
2. [Na] = [Na], K = 1, charge = +1
3. [Cl] = [Cl], K = 1, charge = -1
4. [H] = [H], K = 1, charge = +1
5. [DL] = ? , charge = 0
6. [DOCwH] = [DOCwH], K = 1, charge = 0
7. [DOCsH] = [DOCsH], K = 1, charge = 0
8. [OH] = -1\*[H], Kw = 10^-13.997, charge = -1
9. [CuOH] = [Cu] + -1\*[H], KCuOH = 10^-7.52, charge = +1
10. [CuCl] = [Cu] + [Cl], K = 10^0.4, charge = +1
11. [DL-Cu] = 2\*[DL] + [Cu], K = 1, charge = +2
12. [DL-Na] = [DL] + [Na], K = 1, charge = +1
13. [DL-Cl] = [DL] + [Cl], K = 1, charge = -1
14. [DL-H] = [DL] + [H], K = 1, charge = +1
15. [DL-OH] = [DL] + -1\*[H], K = 10-13.997, charge = -1
16. [DL-CuOH] = [DL] + [Cu] + -1\*[H], K=10^-7.52, charge = +1
17. [DL-CuCl] = [DL] + [Cu] + [Cl], K = 10^0.4, charge = +1
18. [DOCw] = [DOCwH] + -1\*[H], K = 10^-1.59, charge = -1
19. [DOCs] = [DOCsH] + -1\*[H], K = 10^-12.4, charge = -1
20. [DOCw-Cu] = [DOCwH] + -1\*[H] + [Cu], K = 10^-0.8, charge = +1
21. [DOCs-Cu] = [DOCsH] + -1\*[H] + [Cu], K = 10^-3.168, charge = +1
22. [DOCw-CuOH] = [DOCwH] + -2\*[H] + [Cu], K = 10-8.32, charge = 0
23. [DOCs-CuOH] = [DOCsH] + -2\*[H] + [Cu], K = 10-10.688, charge = 0

Species Equations:

1. [Cu] = [Cu]
2. [Na] = [Na]
3. [Cl] = [Cl]
4. [H] = [H]
5. [DL] = ?
6. [DOCwH] = [DOCwH]
7. [DOCsH] = [DOCsH]
8. [OH] = [H]-1\*10^-13.997
9. [CuOH] = [Cu]\*[H]-1\*10^-7.52
10. [CuCl] = [Cu]\*[Cl]\*10^0.4
11. [DL-Cu] = [DL]^2\*[Cu]
12. [DL-Na] = [DL]\*[Na]
13. [DL-Cl] = [DL]\*[Cl]
14. [DL-H] = [DL]\*[H]
15. [DL-OH] = [DL]\*[H]-1\*10^-13.997
16. [DL-CuOH] = [DL]\*[Cu]\*[H]-1\*10^-7.52
17. [DL-CuCl] = [DL]\*[Cu]\*[Cl]\*10^0.4
18. [DOCw] = [DOCwH]\*[H]-1\*10^-1.59
19. [DOCs] = [DOCsH] \*[H]-1\*10^-12.4
20. [DOCw-Cu] = [DOCwH]\*[H]-1\*[Cu]\*10^-0.8
21. [DOCs-Cu] = [DOCsH]\*[H]-1 \*[Cu]\*10^-3.168
22. [DOCw-CuOH] = [DOCwH]\*[H]-2\*[Cu]\*10^-8.32
23. [DOCs-CuOH] = [DOCsH]\*[H]-2\*[Cu]\*10^-10.688

Totals (in terms of species concentrations):

* 1. 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
  2. T.Na = [Na]\*Msol + [DL-Na]\*MDL
  3. T.Cl = [Cl]\*Msol + [CuCl]\*Msol + [DL-Cl]\*MDL + [DL-CuCl]\*MDL
  4. 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
  5. T.DL = 2\*[DL-Cu]\*MDL + [DL-Na]\*MDL + [DL-Cl]\*MDL + [DL-H]\*MDL + [DL-OH]\*MDL + [DL-CuOH]\*MDL + [DL-CuCl]\*MDL
  6. T.DOCwH = [DOCwH]\*Msol + [DOCw]\*Msol + [DOCw-Cu]\*Msol + [DOCw-CuOH]\*Msol
  7. T.DOCsH = [DOCsH]\*Msol + [DOCs]\*Msol + [DOCs-Cu]\*Msol + [DOCs-CuOH]\*Msol

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

* 1. 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
  2. T.Na = [Na]\*Msol + [DL]\*[Na]\*MDL
  3. T.Cl = [Cl]\*Msol + [Cu]\*[Cl]\*100.4\*Msol + [DL]\*[Cl]\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL
  4. 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
  5. 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
  6. 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
  7. 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 species):

R.Cu = T.Cu– T.Cuknown

R.Na = T.Na – T.Na­known

R.Cl = T.Cl – T.Clknown

R.H = 0

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

R.DOCwH = T.DOCwH – T.DOCwHknown

R.DOCsH = T.DOCsH – T.DOCsHknown

Residuals (in terms of components):

1. 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
2. R.Na = [Na]\*Msol + [DL]\*[Na]\*MDL – T.Na­known
3. R.Cl = [Cl]\*Msol + [Cu]\*[Cl]\*100.4\*Msol + [DL]\*[Cl]\*MDL + [DL]\*[Cu]\*[Cl]\*100.4\*MDL – T.Clknown
4. R.H = 0
5. 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
6. R.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.DOCwHknown
7. R.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 – T.DOCsHknown

Derivatives:

Jacobian: