

RATES

Calcite

-start

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1  rem M=current number of moles of Calcite
2  rem M0=number of moles of Calcite initially present
3  rem PARM(1) = A/V, cm^2/L
4  rem PARM(2) = exponent for M/M0
10 si_cc = SI("Calcite")
20 if (M <= 0 and si_cc < 0) then goto 200
30 k1 = 10^(0.198-44.0/TK)
40 k2 = 10^(2.84-2177.0/TK)
50 if TC <= 25 then k3 = 10^(-5.86-317.0/TK)
60 if TC > 25 then k3 = 10^(-1.1-1737.0/TK)
70 t = 1
80 if M0 > 0 then t = M/M0
90 if t = 0 then t = 1
100 area = PARM(1) * (t)^PARM(2)
110 rf = k1*ACT("H+") + k2*ACT("CO2") + k3*ACT("H2O")
120 rem 1e-3 converts mmol to mol
130 rate = area * 1e-3 * rf * (1 - 10^(2/3*si_cc))
140 moles = rate * TIME
200 SAVE moles
-end
```

KINETICS

Calcite

-parms 127 0.67

-m0 0

-m 0