Adsorption in Daisy

Python interface
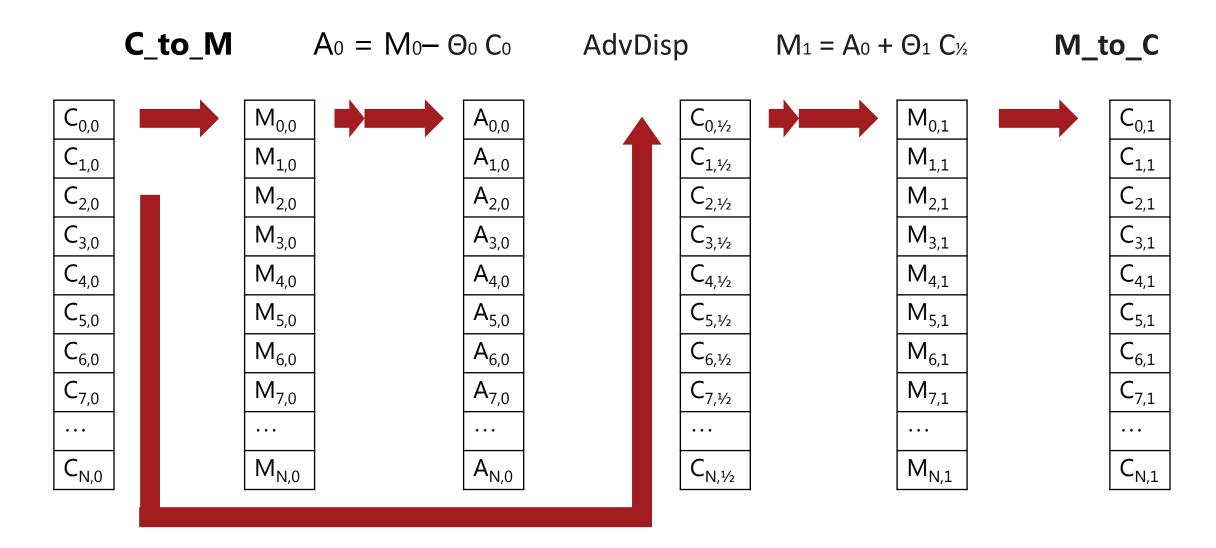
Per Abrahamsen

UNIVERSITY OF COPENHAGEN

Adsorption and solute transport

C_to_M $\qquad$ $A_0 = M_0 - \Theta_0 C_0$ $\qquad$ AdvDisp $\qquad$ $M_1 = A_0 + \Theta_1 C_{\frac{1}{2}}$ $\qquad$ **M_to_C**

$C_{0,0}$	$M_{0,0}$	$A_{0,0}$	$C_{0,\frac{1}{2}}$	$M_{0,1}$	$C_{0,1}$
$C_{1,0}$	$M_{1,0}$	$A_{1,0}$	$C_{1,\frac{1}{2}}$	$M_{1,1}$	$C_{1,1}$
$C_{2,0}$	$M_{2,0}$	$A_{2,0}$	$C_{2,\frac{1}{2}}$	$M_{2,1}$	$C_{2,1}$
$C_{3,0}$	$M_{3,0}$	$A_{3,0}$	$C_{3,\frac{1}{2}}$	$M_{3,1}$	$C_{3,1}$
$C_{4,0}$	$M_{4,0}$	$A_{4,0}$	$C_{4,\frac{1}{2}}$	$M_{4,1}$	$C_{4,1}$
$C_{5,0}$	$M_{5,0}$	$A_{5,0}$	$C_{5,\frac{1}{2}}$	$M_{5,1}$	$C_{5,1}$
$C_{6,0}$	$M_{6,0}$	$A_{6,0}$	$C_{6,\frac{1}{2}}$	$M_{6,1}$	$C_{6,1}$
$C_{7,0}$	$M_{7,0}$	$A_{7,0}$	$C_{7,\frac{1}{2}}$	$M_{7,1}$	$C_{7,1}$
…	…	…	…	…	…
$C_{N,0}$	$M_{N,0}$	$A_{N,0}$	$C_{N,\frac{1}{2}}$	$M_{N,1}$	$C_{N,1}$

Linear adsorption

test-MySorb.dai

```
(defadsorption MySorb Python
  "Use Python for sorption."
  (module "daisy")
  (C_to_M "C_to_M")
  (M_to_C "M_to_C")) ; Optional

(defchemical MyStuff classic
  (decompose_rate 0)
  (adsorption MySorb))

(defchemistry MyChem default
  (trace MyStuff))
```

daisy.py

```python
def k_soil (f_OC, f_clay):
    k_OC = 44.1
    k_clay = 9.2
    return f_OC * k_OC + f_clay * k_clay

def C_to_M (C, Theta_sat, Theta, rho_b, f_OC, f_clay, d50, T):
    k = k_soil (f_OC, f_clay)
    M = rho_b * k * C + Theta * C
    return M

def M_to_C (M, Theta_sat, Theta, rho_b, f_OC, f_clay, d50, T):
    k = k_soil (f_OC, f_clay)
    # M = rho_b * k * C + Theta * C =>
    C = M / (rho_b * k + Theta)
    return C
```

Parameters

Name	Unit	Description
C	g/cm^3	Concentration in water
M	g/cm^3	Concentration in system
Theta_sat	cm^3/cm^3	Saturated volumetric water content
Theta	cm^3/cm^3	Actual volumetric water content
rho_b	g/cm^3	Dry bulk density (soil weight per system volume)
f_OC	0-1	Fraction of organic carbon in soil
f_clay	0-1	Fraction clay of in soil
d50	µm	Median diameter of oil particles by weight
T	°C	Soil temperature