

Implementation of CLM Below-Ground Biogeochemistry in PFLOTRAN

July 30, 2013

Abstract

1 CLM-CN

1.1 Reactions

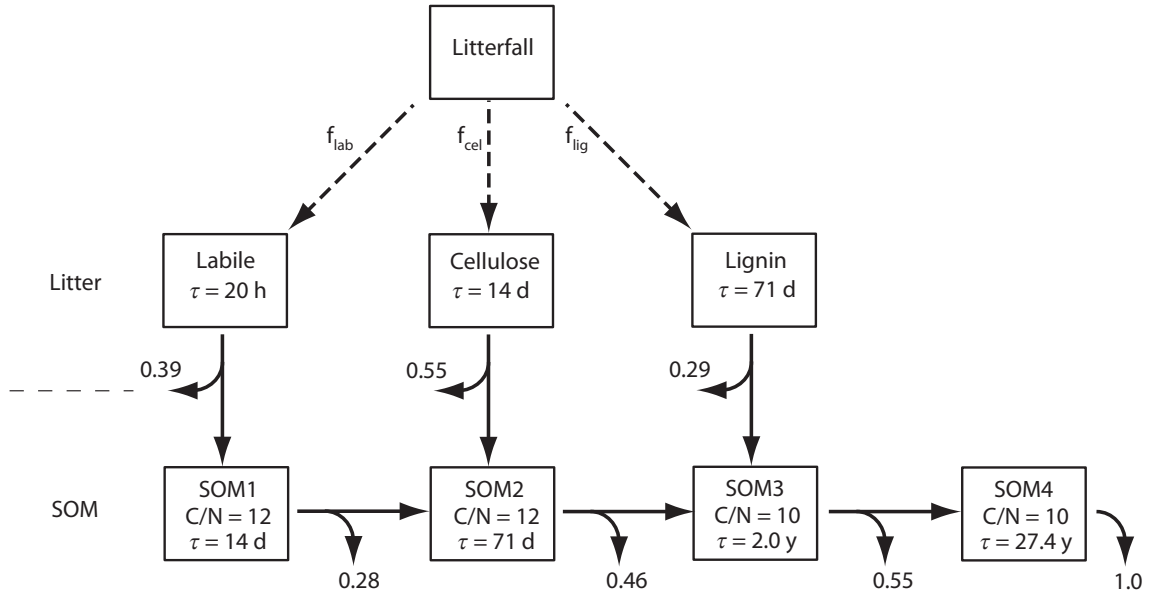


Figure 1: CLM-CN litter and soil organic pools and C and N flows Bonan et al. [2012]

1.1.1 General Reaction

The general decomposition reaction is

$$CN_u = (1 - f)CN_d + fCO_2 + nN_{\text{mineral}} \quad (1)$$

CN_u	=	upstream pool
CN_d	=	downstream pool
CO_2	=	
N_{mineral}	=	mineral nitrogen
u	=	molecular weight ratio of C and N divided by upstream pool C/N
d	=	molecular weight ratio of C and N divided by downstream pool C/N
f	=	respiration fraction
n	=	$[u - (1 - f)d]$

1.1.2 Soil Organic Matter Pools

The C/N ratio is fixed in soil organic matter pools. The reactions are

Table 1: Reactions for the soil organic matter pools

SOM1	=	$0.72 \text{ SOM2} + 0.28 \text{ CO}_2 + 0.020000 \text{ N}_{\text{mineral}}$
SOM2	=	$0.54 \text{ SOM3} + 0.46 \text{ CO}_2 + 0.025143 \text{ N}_{\text{mineral}}$
SOM3	=	$0.45 \text{ SOM4} + 0.55 \text{ CO}_2 + 0.047143 \text{ N}_{\text{mineral}}$
SOM4	=	$\text{CO}_2 + 0.085714 \text{ N}_{\text{mineral}}$

1.1.3 Litter Pools

The C/N ratio is dependent on the input from plant function groups. As the C/N ratio is generally greater in the litter pools than in the soil organic pools Adair et al. [2008], mineral N is needed to decompose the litter pools. Namely, litter decomposition involves N immobilization through microbial mass synthesis. For example, one observation indicates a C/N ratio of 31.19 for yellow birch Adair et al. [2008]. The reactions are

Table 2: Reactions for the litter pools

$\text{Lit1C} + 0.027481 \text{ Lit1N} + 0.016090 \text{ N}_{\text{mineral}}$	=	$0.61 \text{ SOM1} + 0.39 \text{ CO}_2$
$\text{Lit2C} + 0.027481 \text{ Lit2N} + 0.004662 \text{ N}_{\text{mineral}}$	=	$0.45 \text{ SOM2} + 0.55 \text{ CO}_2$
$\text{Lit3C} + 0.027481 \text{ Lit3N} + 0.033376 \text{ N}_{\text{mineral}}$	=	$0.71 \text{ SOM3} + 0.29 \text{ CO}_2$

1.1.4 Summary

$$\begin{aligned}
\text{Lit1C} + u_1 \text{Lit1N} &= (1 - f_1) \text{SOM1} + f_1 \text{CO}_2 + n_1 \text{N}_{\text{mineral}} \\
\text{Lit2C} + u_2 \text{Lit2N} &= (1 - f_2) \text{SOM2} + f_2 \text{CO}_2 + n_2 \text{N}_{\text{mineral}} \\
\text{Lit3C} + u_3 \text{Lit3N} &= (1 - f_3) \text{SOM3} + f_3 \text{CO}_2 + n_3 \text{N}_{\text{mineral}} \\
\text{SOM1} &= (1 - f_4) \text{SOM2} + f_4 \text{CO}_2 + n_4 \text{N}_{\text{mineral}} \\
\text{SOM2} &= (1 - f_5) \text{SOM3} + f_5 \text{CO}_2 + n_5 \text{N}_{\text{mineral}} \\
\text{SOM3} &= (1 - f_6) \text{SOM4} + f_6 \text{CO}_2 + n_6 \text{N}_{\text{mineral}} \\
\text{SOM4} &= f_7 \text{CO}_2 + n_7 \text{N}_{\text{mineral}}
\end{aligned}$$

$$u_i = \text{LitiN}/\text{LitiC}$$

1.2 Rate

1.2.1 General

$$rate = R = f_T f_\Psi f_N k \text{CN}_u \quad (2)$$

$$f_T = \exp \left[308.56 \left(\frac{1}{71.02} - \frac{1}{T - 227.13} \right) \right]$$

$$f_\Psi = \frac{\log(\Psi_{\min}/\Psi)}{\log(\Psi_{\min}/\Psi_{\max})}$$

$$f_{\text{pi}} = \frac{\text{N}_{\text{mineral}}}{\text{N}_{\text{mineral}} + k_{\text{N}_{\text{mineral}}}} \text{if } u$$

$$k = \text{kinetic rate constant} [s^{-1}]$$

$$T = \text{temperature} [K]$$

$$\Psi = \text{soil water potential} [MPa]$$

$$\text{CN}_u = \text{upstream carbon pool} [\text{mol C}/m^3]$$

$$\text{N}_{\text{mineral}} = \text{nitrogen concentration} [\text{mol N}/m^3]$$

$$k_N = \text{Mineral N half saturation constant} [\text{mol N}/m^3]$$

For the general reaction 1,

$$\begin{aligned}
\frac{\partial \text{CN}_u}{\partial t} &= -rate \\
\frac{\partial \text{CN}_d}{\partial t} &= (1 - f) rate \\
\frac{\partial \text{CO}_2}{\partial t} &= f \cdot rate \\
\frac{\partial \text{N}_{\text{mineral}}}{\partial t} &= n \cdot rate
\end{aligned}$$

1.2.2 Rates

$$\begin{aligned}
R_1 &= f_T f_\theta f_N k_1 \text{Lit1C} \\
R_2 &= f_T f_\theta f_N k_2 \text{Lit2C} \\
R_3 &= f_T f_\theta f_N k_3 \text{Lit3C} \\
R_4 &= f_T f_\theta f_N k_4 \text{SOM1} \\
R_5 &= f_T f_\theta f_N k_5 \text{SOM2} \\
R_6 &= f_T f_\theta f_N k_6 \text{SOM3} \\
R_7 &= f_T f_\theta f_N k_7 \text{SOM4}
\end{aligned}$$

1.2.3 Ordinary Differential Equations

$$\begin{aligned}
\frac{\partial}{\partial t} (\text{Lit1C}) &= -R_1 \\
\frac{\partial}{\partial t} (\text{Lit1N}) &= -u_1 R_1 \\
\frac{\partial}{\partial t} (\text{Lit2C}) &= -R_2 \\
\frac{\partial}{\partial t} (\text{Lit3N}) &= -u_2 R_2 \\
\frac{\partial}{\partial t} (\text{Lit3C}) &= -R_3 \\
\frac{\partial}{\partial t} (\text{Lit3N}) &= -u_3 R_3 \\
\frac{\partial}{\partial t} (\text{SOM1}) &= (1 - f_1) R_1 - R_4 \\
\frac{\partial}{\partial t} (\text{SOM2}) &= (1 - f_2) R_2 + (1 - f_4) R_4 - R_5 \\
\frac{\partial}{\partial t} (\text{SOM3}) &= (1 - f_3) R_3 + (1 - f_5) R_5 - R_6 \\
\frac{\partial}{\partial t} (\text{SOM4}) &= (1 - f_6) R_6 - R_7 \\
\frac{\partial}{\partial t} (\text{CO}_2) &= f_1 R_1 + f_2 R_2 + f_3 R_3 + f_4 R_4 + f_5 R_5 + f_6 R_6 + f_7 R_7 \\
\frac{\partial}{\partial t} (\text{N}_{\text{mineral}}) &= n_1 R_1 + n_2 R_2 + n_3 R_3 + n_4 R_4 + n_5 R_5 + n_6 R_6 + n_7 R_7
\end{aligned}$$

1.3 Implementation in PFLOTTRAN

1.3.1 Numerical Methods

Applying finite-volume spatial discretization:

$$\int \frac{\partial x}{\partial t} dV = \int - \sum R_j dV \tag{3}$$

$$\frac{\partial x}{\partial t} \Delta V = - \sum R_j \Delta V \quad (4)$$

Implicit time discretization:

$$\frac{\Delta V}{\Delta t} (x^{k+1} - x^k) = - \sum R_j^{k+1} \Delta V \quad (5)$$

Residual equation:

$$\mathcal{R}_x = \frac{\Delta V}{\Delta t} (x^{k+1} - x^k) + \sum R_i^{k+1} \Delta V \quad (6)$$

Newton-Raphson Method:

$$\mathcal{J} \delta x = -\mathcal{R}_x \quad (7)$$

$$x^{k+1,i+1} = x^{k+1,i} + \delta x \quad (8)$$

1.3.2 Implementation

The source code `reaction_sandbox_clm_cn.F90` implements CLM-CN with input file like the following:

CHEMISTRY

...

IMMOBILE_SPECIES

N

C

SOM1

SOM2

SOM3

SOM4

LabileC

CelluloseC

LigninC

LabileN

CelluloseN

LigninN

/

...

REACTION_SANDBOX

CLM-CN

POOLS ! CN ratio

SOM1 12.d0

SOM2 12.d0

SOM3 10.d0

SOM4 10.d0

Labile

```

    Cellulose
    Lignin
/
REACTION
    UPSTREAM_POOL Labile
    DOWNSTREAM_POOL SOM1
    TURNOVER_TIME 20. h
    RESPIRATION_FRACTION 0.39d0
    N_INHIBITION 1.d-10
/
REACTION
    UPSTREAM_POOL Cellulose
    DOWNSTREAM_POOL SOM2
    TURNOVER_TIME 14. d
    RESPIRATION_FRACTION 0.55
    N_INHIBITION 1.d-10
/
REACTION
    UPSTREAM_POOL Lignin
    DOWNSTREAM_POOL SOM3
    TURNOVER_TIME 71. d
    RESPIRATION_FRACTION 0.29d0
    N_INHIBITION 1.d-10
/
REACTION
    UPSTREAM_POOL SOM1
    DOWNSTREAM_POOL SOM2
    TURNOVER_TIME 14. d
    RESPIRATION_FRACTION 0.28d0
    N_INHIBITION 1.d-10
/
REACTION
    UPSTREAM_POOL SOM2
    DOWNSTREAM_POOL SOM3
    TURNOVER_TIME 71. d
    RESPIRATION_FRACTION 0.46d0
    N_INHIBITION 1.d-10
/
REACTION
    UPSTREAM_POOL SOM3
    DOWNSTREAM_POOL SOM4
    TURNOVER_TIME 2. y
    RESPIRATION_FRACTION 0.55d0
    N_INHIBITION 1.d-10
/
REACTION

```

```

UPSTREAM_POOL SOM4
TURNOVER_TIME 27.4 y
RESPIRATION_FRACTION 1.d0
N_INHIBITION 1.d-10
/
/
/
/

```

In the source code, the key is to specify the residual and Jacobian. The residuals are:

$$\begin{aligned}
\mathcal{R}_{\text{Lit1C}} &= \frac{\Delta V}{\Delta t} (\text{Lit1C}^{k+1} - \text{Lit1C}^k) + R_1^{k+1} \Delta V \\
\mathcal{R}_{\text{Lit1N}} &= \frac{\Delta V}{\Delta t} (\text{Lit1N}^{k+1} - \text{Lit1N}^k) + u_1 R_1^{k+1} \Delta V \\
\mathcal{R}_{\text{Lit2C}} &= \frac{\Delta V}{\Delta t} (\text{Lit2C}^{k+1} - \text{Lit2C}^k) + R_2^{k+1} \Delta V \\
\mathcal{R}_{\text{Lit2N}} &= \frac{\Delta V}{\Delta t} (\text{Lit2N}^{k+1} - \text{Lit2N}^k) + u_2 R_2^{k+1} \Delta V \\
\mathcal{R}_{\text{Lit3C}} &= \frac{\Delta V}{\Delta t} (\text{Lit3C}^{k+1} - \text{Lit3C}^k) + R_3^{k+1} \Delta V \\
\mathcal{R}_{\text{Lit3N}} &= \frac{\Delta V}{\Delta t} (\text{Lit3N}^{k+1} - \text{Lit3N}^k) + u_3 R_3^{k+1} \Delta V \\
\mathcal{R}_{\text{SOM1}} &= \frac{\Delta V}{\Delta t} (\text{SOM1}^{k+1} - \text{SOM1}^k) - [(1 - f_1)R_1^{k+1} - R_4^{k+1}] \Delta V \\
\mathcal{R}_{\text{SOM2}} &= \frac{\Delta V}{\Delta t} (\text{SOM2}^{k+1} - \text{SOM2}^k) - [(1 - f_2)R_2^{k+1} + (1 - f_4)R_4^{k+1} - R_5^{k+1}] \Delta V \\
\mathcal{R}_{\text{SOM3}} &= \frac{\Delta V}{\Delta t} (\text{SOM3}^{k+1} - \text{SOM3}^k) - [(1 - f_3)R_3^{k+1} + (1 - f_5)R_5^{k+1} - R_6^{k+1}] \Delta V \\
\mathcal{R}_{\text{SOM4}} &= \frac{\Delta V}{\Delta t} (\text{SOM4}^{k+1} - \text{SOM4}^k) - [(1 - f_6)R_6^{k+1} - R_7^{k+1}] \Delta V \\
\mathcal{R}_{\text{CO}_2} &= \frac{\Delta V}{\Delta t} (\text{CO}_2^{k+1} - \text{CO}_2^k) \\
&\quad - [f_1 R_1^{k+1} + f_2 R_2^{k+1} + f_3 R_3^{k+1} + f_4 R_4^{k+1} + f_5 R_5^{k+1} + f_6 R_6^{k+1} + R_7^{k+1}] \Delta V \\
\mathcal{R}_{\text{N}_{\text{mineral}}} &= \frac{\Delta V}{\Delta t} (\text{N}_{\text{mineral}}^{k+1} - \text{N}_{\text{mineral}}^k) \\
&\quad - [n_1 R_1^{k+1} + n_2 R_2^{k+1} + n_3 R_3^{k+1} + n_4 R_4^{k+1} + n_5 R_5^{k+1} + n_6 R_6^{k+1} + R_7^{k+1}] \Delta V
\end{aligned}$$

For Lit1 decomposition, the rate is

$$R_1 = f_T f_\Psi f_N k_1 \text{Lit1C} \quad (9)$$

the derivatives are:

$$\frac{\partial R_1}{\partial \text{Lit1C}} = f_T f_\Psi f_N k_1 = R'_{1, \text{Lit1C}} \quad (10)$$

$$\frac{\partial R_1}{\partial \text{N}_{\text{mineral}}} = f_T f_\Psi k_1 \text{Lit1C} \frac{k_N}{(k_N + \text{N}_{\text{mineral}})^2} = R'_{1, \text{N}} \quad (11)$$

$$\begin{aligned}
\frac{\partial R_{\text{Lit1N}}}{\partial \text{Lit1C}} &= \frac{\partial(u_1 R_1)}{\partial \text{Lit1C}} = R_1 \frac{\partial u_1}{\partial \text{Lit1C}} + u_1 R_{1,\text{Lit1C}} = -R_1 \frac{\text{Lit1N}}{\text{Lit1C}^2} + u_1 R'_{1,\text{Lit1C}} \\
\frac{\partial R_{\text{Lit1N}}}{\partial R_{\text{Lit1C}}} &= \frac{\partial(u_1 R_1)}{\partial(u_1 R_1)} = R_1 \frac{\partial u_1}{\partial \text{Lit1N}} = R_1 \frac{1}{\text{Lit1C}} \\
\frac{\partial R_{\text{Lit1N}}}{\partial N_{\text{mineral}}} &= \frac{\partial(u_1 R_1)}{\partial N_{\text{mineral}}} = R_1 \frac{\partial u_1}{\partial N_{\text{mineral}}} + u_1 R'_{1,N} = u_1 R'_{1,N} \\
\frac{\partial R_{N_{\text{mineral}}}}{\partial \text{Lit1C}} &= -\frac{\partial \text{Lit1C}}{\partial(n_1 R_1)} = -R_1 \frac{\partial n_1}{\partial \text{Lit1C}} - n_1 R'_{1,\text{Lit1C}} = R_1 \frac{\text{Lit1N}}{\text{Lit1C}^2} - n_1 R'_{1,\text{Lit1C}} \\
\frac{\partial R_{N_{\text{mineral}}}}{\partial R_{\text{Lit1C}}} &= -\frac{\partial \text{Lit1C}}{\partial(n_1 R_1)} = -R_1 \frac{\partial n_1}{\partial \text{Lit1C}} = -R_1 \frac{1}{\text{Lit1C}} \\
\frac{\partial R_{N_{\text{mineral}}}}{\partial \text{Lit1N}} &= -\frac{\partial \text{Lit1N}}{\partial(n_1 R_1)} = -R_1 \frac{\partial n_1}{\partial \text{Lit1N}} = -n_1 R'_{1,N} \\
\frac{\partial R_{N_{\text{mineral}}}}{\partial N_{\text{mineral}}} &= -\frac{\partial(n_1 R_1)}{\partial N_{\text{mineral}}} = -R_1 \frac{\partial n_1}{\partial N_{\text{mineral}}} = -n_1 R'_{1,N}
\end{aligned}$$

Table 3: Jacobian for Litter Pools

	LitiC	LitiN	SOMi	CO ₂	N _{mineral}
LitiC	$R'_{i,\text{LitiC}}$	0	0	0	$R'_{i,N}$
LitiN	$-R_i \frac{\text{Lit1N}}{\text{Lit1C}^2} + u_i R'_{i,\text{LitiC}}$	$R_i \frac{1}{\text{Lit1C}}$	0	0	$u_i R'_{i,N}$
SOMi	$-(1 - f_i) R'_{i,\text{LitiC}}$	0	0	0	$-(1 - f_i) R'_{i,N}$
CO ₂	$-f_i R'_{i,\text{LitiC}}$	0	0	0	$-f_i R'_{i,N}$
N _{mineral}	$R_i \frac{\text{Lit1N}}{\text{Lit1C}^2} - n_i R'_{i,\text{LitiC}}$	$-R_i \frac{1}{\text{Lit1C}}$	0	0	$-n_i R'_{i,N}$

Table 4: Jacobian for SOM Pools

	SOM1	SOM2	SOM3	SOM4	CO ₂	N _{mineral}
SOM1	R'_4	0	0	0	0	0
SOM2	$-(1 - f_4) R'_4$	R'_5	0	0	0	0
SOM3	0	$-(1 - f_5) R'_5$	R'_6	0	0	0
SOM4	0	0	$-(1 - f_6) R'_6$	R'_7	0	0
CO ₂	$-f_4 R'_4$	$-f_5 R'_5$	$-f_6 R'_6$	$-R'_7$	0	0
N _{mineral}	$-n_4 R'_4$	$-n_5 R'_5$	$-n_6 R'_6$	$-n_7 R'_7$	0	0

1.4 Applications

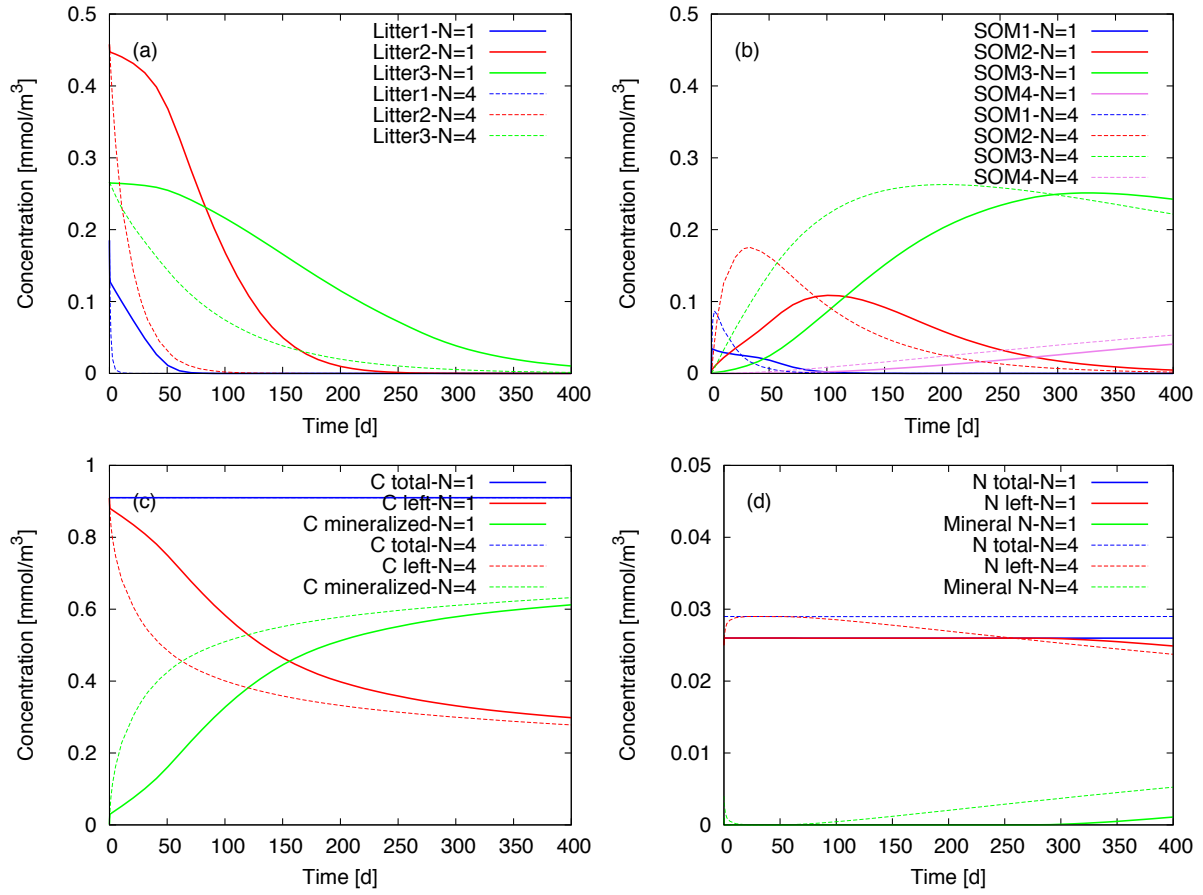


Figure 2: Demonstrating N limiting on C decomposition (initial mineral N=1 and 4 μ mol/m³)

2 CLM4.5 CH₄ Oxidation

2.1 Reaction



2.2 Rate

$$R = k \frac{\text{CH}_4}{k_{\text{CH}_4} + \text{CH}_4} \frac{\text{O}_2}{k_{\text{O}_2} + \text{O}_2} f_T f_\Psi \quad (13)$$

2.3 Residuals

$$\begin{aligned} \mathcal{R}_{\text{CH}_4} &= \frac{\Delta V}{\Delta t} (\text{CH}_4^{k+1} - \text{CH}_4^k) + R^{k+1} \Delta V \\ \mathcal{R}_{\text{O}_2} &= \frac{\Delta V}{\Delta t} (\text{O}_2^{k+1} - \text{O}_2^k) + 2R^{k+1} \Delta V \\ \mathcal{R}_{\text{CO}_2} &= \frac{\Delta V}{\Delta t} (\text{CO}_2^{k+1} - \text{CO}_2^k) - R^{k+1} \Delta V \end{aligned}$$

2.4 Jacobian

$$\begin{aligned} \frac{\partial R}{\partial \text{CH}_4} &= k \frac{k_{\text{CH}_4}}{(k_{\text{CH}_4} + \text{CH}_4)^2} \frac{\text{O}_2}{k_{\text{O}_2} + \text{O}_2} f_T f_\Psi = R'_{\text{CH}_4} \\ \frac{\partial R}{\partial \text{O}_2} &= k \frac{\text{CH}_4}{k_{\text{CH}_4} + \text{CH}_4} \frac{k_{\text{O}_2}}{(k_{\text{O}_2} + \text{O}_2)^2} f_T f_\Psi = R'_{\text{O}_2} \end{aligned}$$

Table 5: Jacobian for methane oxidation

	CH ₄	O ₂	CO ₂
CH ₄	R'_{CH_4}	R'_{O_2}	0
O ₂	$2R'_{\text{CH}_4}$	$2R'_{\text{O}_2}$	0
CO ₂	$-R'_{\text{CH}_4}$	$-R'_{\text{O}_2}$	0

2.5 Application

Input file

```
CHEMISTRY
PRIMARY_SPECIES
O2(aq)
Methane(aq)
CO2(aq)
```

```

/
REDOX_SPECIES
  CO2(aq)
  Methane(aq)
  O2(aq)
/
REACTION_SANDBOX
  CH4O
    RATE_CONSTANT 1.25d-10 ! mol/m3 s
    HALFSATURATIONCH4 5.0d-6
    HALFSATURATIONO2 2.0d-5
  /
/
DATABASE ../../pflotran-clm4me/database/hanford.dat
.....
CONSTRAINT initial
  CONCENTRATIONS
    O2(aq)      0.001 T
    Methane(aq) 0.001 T
    CO2(aq)     1.0d-10 T
  /
END

Code

subroutine CH4OReact(this,Residual,Jacobian,compute_derivative, &
                    rt_auxvar,global_auxvar,porosity,volume,reaction, &
                    option)

  word = "Methane(aq)"
  is_ch4 = GetPrimarySpeciesIDFromName(word,reaction,option)

  word = "CO2(aq)"
  is_co2 = GetPrimarySpeciesIDFromName(word,reaction,option)

  word = "O2(aq)"
  is_o2 = GetPrimarySpeciesIDFromName(word,reaction,option)

  temp_K = global_auxvar%temp(1) + 273.15d0
  F_t = exp(308.56d0*(one_over_71_O2 - 1.d0/(temp_K - 227.13d0)))

  F_theta = log(theta_min/global_auxvar%sat(1)) * one_over_log_theta_min

  L_water = porosity*global_auxvar%sat(iphase)*volume*1.d3
  c_ch4 = rt_auxvar%total(is_ch4,iphase)
  c_o2 = rt_auxvar%total(is_o2,iphase)

  rate = this%rate_constant * L_water * & ! mole/(L sec)

```

```

    c_ch4/(this%kmch4 + c_ch4) * c_o2/(this%kmo2 + c_o2) * F_t * F_theta

Residual(is_ch4) = Residual(is_ch4) + rate
Residual(is_o2) = Residual(is_o2) + 2.0 * rate
Residual(is_co2) = Residual(is_co2) - rate

if (compute_derivative) then

    ! always add contribution to Jacobian
    ! units = (mol/sec)*(kg water/mol) = kg water/sec

    !dx/(k+x) = k/(k+x)^2

    drate_dch4 = rate * this%kmch4 / c_ch4 / (this%kmch4 + c_ch4)
    drate_do2  = rate * this%kmo2 / c_o2 / (this%kmo2 + c_o2)

    Jacobian(is_ch4,is_ch4) = Jacobian(is_ch4,is_ch4) - drate_dch4
    Jacobian(is_ch4,is_o2) = Jacobian(is_ch4,is_o2) - drate_do2
    Jacobian(is_o2,is_ch4) = Jacobian(is_o2,is_ch4) - 2.0 * drate_dch4
    Jacobian(is_o2,is_o2) = Jacobian(is_o2,is_o2) - 2.0 * drate_do2
    Jacobian(is_co2,is_ch4) = Jacobian(is_co2,is_ch4) + drate_dch4
    Jacobian(is_co2,is_o2) = Jacobian(is_co2,is_o2) + drate_do2

endif

end subroutine CH4OReact

```

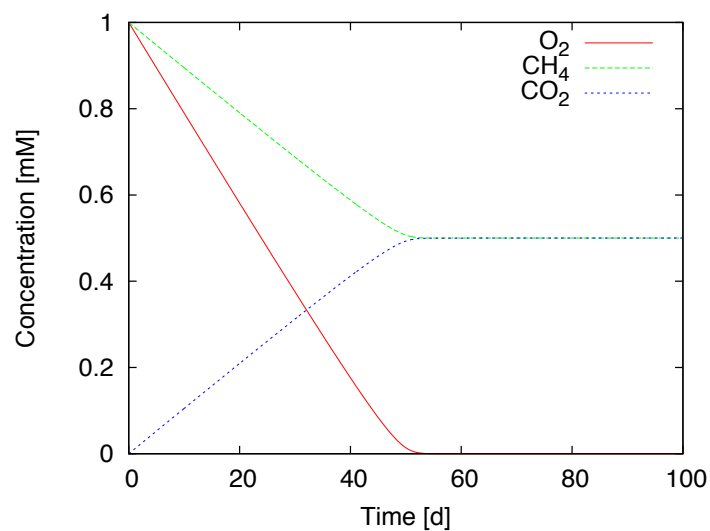


Figure 3: Example calculation for methane oxidation)

3 Acetoclastic Methanogenesis

3.1 Reaction



3.2 Rate

$$R = k\text{C}_{\text{bio}} \frac{\text{Ac}^-}{k_{\text{Ac}} + \text{Ac}^-} f_T f_\Psi \quad (16)$$

3.3 Residuals

$$\begin{aligned} \mathcal{R}_{\text{Ac}^-} &= \frac{\Delta V}{\Delta t} (\text{Ac}^{-k+1} - \text{Ac}^{-k}) + (1 + y/2)R^{k+1}\Delta V \\ \mathcal{R}_{\text{CH}_4} &= \frac{\Delta V}{\Delta t} (\text{CH}_4^{k+1} - \text{CH}_4^k) - R^{k+1}\Delta V \\ \mathcal{R}_{\text{C}_{\text{bio}}} &= \frac{\Delta V}{\Delta t} (\text{C}_{\text{bio}}^{k+1} - \text{C}_{\text{bio}}^k) - yR^{k+1}\Delta V \\ \mathcal{R}_{\text{HCO}_3^-} &= \frac{\Delta V}{\Delta t} (\text{HCO}_3^{-k+1} - \text{HCO}_3^{-k}) - R^{k+1}\Delta V \\ \mathcal{R}_{\text{H}^+} &= \frac{\Delta V}{\Delta t} (\text{H}^{+k+1} - \text{H}^{+k}) + y/2R^{k+1}\Delta V \end{aligned}$$

3.4 Jacobian

$$\begin{aligned} \frac{\partial R}{\partial \text{Ac}^-} &= k\text{C}_{\text{bio}} \frac{k_{\text{Ac}}}{(k_{\text{Ac}} + \text{Ac}^-)^2} f_T f_\Psi = R'_a \\ \frac{\partial R}{\partial \text{C}_{\text{bio}}} &= k \frac{\text{Ac}^-}{k_{\text{Ac}} + \text{Ac}^-} f_T f_\Psi = R'_b \end{aligned}$$

Table 6: Jacobian for methane oxidation

	Ac^-	CH_4	C_{bio}	HCO_3^-	H^+
Ac^-	$(1 + y/2)R'_a$	0	$(1 + y/2)R'_b$	0	0
CH_4	$-R'_a$	0	$-R'_b$	0	0
C_{bio}	$-yR'_a$	0	$-yR'_b$	0	0
HCO_3^-	$-R'_a$	0	$-R'_b$	0	0
H^+	$0.5yR'_a$	0	$0.5yR'_b$	0	0

References

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