Implementation of CLM-CNP in PFLOTRAN

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Abstract

1 Introduction

Starting from CLM-CN, CLM-CNP provides options to

1. add microbial, enzyme, and DOC pools
2. allow variable C:N:P ratios in all of the pools
3. use Monod, Machielis-Menten and other rate models
4. specify immobile or mobile pools/species

through an input file. It reduces to CLM-CN if none of the additional features is specified in the input file. These added features can be added incrementally. Sorption, and other geochemical processes can be added separately (outside of the CLM-CNP reaction_sandbox).

1.1 C

1.1.1 Reaction

$$\mathrm{C}_u \rightarrow c_m\mathrm{C}_m + c_b\mathrm{C}_b + c_e\mathrm{C}_e + c_d\mathrm{C}_d \tag{1}$$

or

$$\mathrm{C}_u \rightarrow \sum c_i\mathrm{C}_i \tag{2}$$

The subscript u, m, b, e, and d denote upstream, mineral, bacterial, enzyme, and downstream pools. To balance the reaction, $c_m + c_b + c_e + c_d = 1$. c_b and c_e can be variable in the future.

For CLM-CN, c_m is the respiration fraction f, $c_d = 1 - f$, and $c_b = c_e = 0$.

To incorporate microbial pools with Monod rate, $c_b \neq 0$.

To use Michaelis-Menten rate, $c_e \neq 0$

1.1.2 Rate

$$\frac{d[\mathrm{C}_u]}{dt} = -R = -k\prod f([\mathrm{C}_i])f(pH)f(\psi)f(T) \tag{3}$$

$[\mathrm{C}_i]$ is the concentration of C_i. k is the rate coefficient. function $f([\mathrm{C}_i])$, $f(pH)$, $f(\psi)$, and $f(T)$ account for influence of C_i, pH, moisture, and temperature on the reaction rate. C_i can be any component in or not in Eq. (1). We consider four options for $f([\mathrm{C}_i])$:

$f([\mathrm{C}_i]) = 1$	default
$f([\mathrm{C}_i]) = [\mathrm{C}_i]$	first order
$f([\mathrm{C}_i]) = [\mathrm{C}_i]/(K_{Ci} + [\mathrm{C}_i])$	substrate/electron donor or electron acceptor limitation
$f([\mathrm{C}_i]) = I_{Ci}/(I_{Ci} + [\mathrm{C}_i])$	inhibition

For CLM-CN, $f([\mathrm{C}_u]) = [\mathrm{C}_u]$, $f([\mathrm{C}_m]) = f([\mathrm{C}_b]) = f([\mathrm{C}_d]) = 1$.

To incorporate microbial pools without Monod rate, $f([\mathrm{C}_u]) = [\mathrm{C}_u]/(K_{C_u} + [\mathrm{C}_u])$, $f([\mathrm{C}_b]) = [\mathrm{C}_b]$, $f([\mathrm{C}_m]) = f([\mathrm{C}_d]) = 1$.

To use Michaelis-Menten rate, $f([\mathrm{C}_u]) = [\mathrm{C}_u]/(K_{C_u} + [\mathrm{C}_u])$, $f([\mathrm{C}_e]) = [\mathrm{C}_e]$, $f([\mathrm{C}_m]) = f([\mathrm{C}_d]) = f([\mathrm{C}_b]) = 1$.

1.2 N

1.2.1 Reaction

$$n_u\mathrm{N}_u \rightarrow n_m\mathrm{N}_m + n_b\mathrm{N}_b + n_e\mathrm{N}_e + n_d\mathrm{N}_d \tag{4}$$

or

$$n_u\mathrm{N}_u \rightarrow \sum n_i\mathrm{N}_i \tag{5}$$

$$n_m + n_b + n_e + n_d = n_u \tag{6}$$

$n_u = [\mathrm{N}_u]/[\mathrm{C}_u]$, $n_b = [\mathrm{N}_b]/[\mathrm{C}_b]$, $n_e = [\mathrm{N}_e]/[\mathrm{C}_e]$, and $n_d = [\mathrm{N}_d]/[\mathrm{C}_d]$. These stoichiometric coefficient can be fixed or variable. If $n_m > 0$, this decomposition reaction produces mineral N (mineralization). Otherwise, the reaction takes up mineral N (immobilization). In the late case, a $f([\mathrm{N}_m]) = [\mathrm{N}_m]/(K_{Nm} + [\mathrm{N}_m])$ term is added tothe decomposition rate in Eq. (3).

1.2.2 Rate

$$-\frac{1}{n_u}\frac{\partial[\mathrm{N}_u]}{\partial t} = \frac{1}{n_m}\frac{\partial[\mathrm{N}_m]}{\partial t} = \frac{1}{n_b}\frac{\partial[\mathrm{N}_b]}{\partial t} = \frac{1}{n_e}\frac{\partial[\mathrm{N}_e]}{\partial t} = \frac{1}{n_d}\frac{\partial[\mathrm{N}_d]}{\partial t} \tag{7}$$

1.3 P

1.3.1 Reaction

$$p_u\mathrm{P}_u \rightarrow p_m\mathrm{P}_m + p_b\mathrm{P}_b + p_e\mathrm{P}_e + p_d\mathrm{P}_d \tag{8}$$

$$p_u\mathrm{P}_u \rightarrow \sum p_i\mathrm{P}_i \tag{9}$$

$$p_m + p_b + p_e + p_d = p_u \tag{10}$$

$p_u = [\mathrm{P}_u]/[\mathrm{C}_u]$, $p_b = [\mathrm{P}_b]/[\mathrm{C}_b]$, $p_e = [\mathrm{P}_e]/[\mathrm{C}_e]$, and $p_d = [\mathrm{P}_d]/[\mathrm{C}_d]$. These stoichiometric coefficient can be fixed or variable. If $p_m > 0$, this decomposition reaction produces mineral P (mineralization). Otherwise, the reaction takes up mineral P (immobilization). In the late case, a $f([\mathrm{P}_m]) = [\mathrm{P}_m]/(K_{Pm} + [\mathrm{P}_m])$ term is added tothe decomposition rate in Eq. (3).

1.3.2 Rate

$$-\frac{1}{p_u}\frac{\partial[\mathrm{P}_u]}{\partial t} = \frac{1}{p_m}\frac{\partial[\mathrm{P}_m]}{\partial t} = \frac{1}{p_b}\frac{\partial[\mathrm{P}_b]}{\partial t} = \frac{1}{p_e}\frac{\partial[\mathrm{P}_e]}{\partial t} = \frac{1}{p_d}\frac{\partial[\mathrm{P}_d]}{\partial t} \tag{11}$$

1.4 Residuals

$$\begin{aligned}
R_{Cu} &= -R \\
R_{Cdi} &= d_i R \\
R_{Cm} &= (1 - d_i) R \\
R_{Nu} &= -\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} R \\
R_{Ndi} &= \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]} R \\
R_{Nm} &= \left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right) R \\
R_{Pu} &= -\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} R \\
R_{Pdi} &= \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]} R \\
R_{Pm} &= \left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right) R
\end{aligned}$$

1.5 Jacobians

Table 1: Jacobian for general decomposition

	C_u	C_{di}	C_m	N_u	N_{di}	N_m	P_u	P_{di}	P_m
C_u	$-\frac{\partial R}{\partial \mathrm{C}_u}$	$-\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$-\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$-\frac{\partial R}{\partial \mathrm{P}_m}$
C_{di}	$d_i\frac{\partial R}{\partial \mathrm{C}_u}$	$d_i\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$d_i\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$d_i\frac{\partial R}{\partial \mathrm{P}_m}$
C_m	$(1-d_i)\frac{\partial R}{\partial \mathrm{C}_u}$	$(1-d_i)\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$(1-d_i)\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$(1-d_i)\frac{\partial R}{\partial \mathrm{P}_m}$
N_u	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_u} + \frac{[\mathrm{N}_u]}{[\mathrm{C}_u]^2}R$	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	$-\frac{1}{[\mathrm{C}_u]}R$	0	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{P}_m}$
N_{di}	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_u}$	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_{di}} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]^2}R$	0	0	$\frac{1}{[\mathrm{C}_{di}]}R$	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{P}_m}$
N_m	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_u} - \frac{[\mathrm{N}_u]}{[\mathrm{C}_u]^2}R$	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_{di}} + \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]^2}R$	0	$\frac{1}{[\mathrm{C}_u]}R$	$-\frac{1}{[\mathrm{C}_{di}]}R$	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{P}_m}$
P_u	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_u} + \frac{[\mathrm{P}_u]}{[\mathrm{C}_u]^2}R$	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{N}_m}$	$-\frac{1}{[\mathrm{C}_u]}R$	0	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{P}_m}$
P_{di}	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_u}$	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_{di}} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]^2}R$	0	0	0	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	$\frac{1}{[\mathrm{C}_{di}]}R$	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{P}_m}$
P_m	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_u} - \frac{[\mathrm{P}_u]}{[\mathrm{C}_u]^2}R$	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_{di}} + \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]^2}R$	0	0	0	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{N}_m}$	$\frac{1}{[\mathrm{C}_u]}R$	$-\frac{1}{[\mathrm{C}_{di}]}R$	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{P}_m}$

To use $\mathrm{N}_m/(\mathrm{K}_N + \mathrm{N}_m)$ term for N-limiting cases ($\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]} < 0$),

$$\frac{\partial R}{\partial \mathrm{N}_m} = R\frac{K_N}{(K_N + \mathrm{N}_m)\mathrm{N}_m} \tag{12}$$

because

$$\frac{\partial \frac{x}{k+x}}{\partial x} = \frac{k}{(k+x)^2} \tag{13}$$

For the first order rate term,

$$\frac{\partial R}{\partial \mathrm{C}_x} = \frac{R}{[\mathrm{C}_x]} \tag{14}$$

For the Monod rate term,

$$\frac{\partial R}{\partial \mathrm{C}_x} = R\frac{K_x}{(K_x + [\mathrm{C}_x])[\mathrm{C}_x]} \tag{15}$$

For the inhibition term,

$$\frac{\partial R}{\partial \mathrm{C}_x} = -R\frac{K_x}{(K_x + [\mathrm{C}_x])[\mathrm{C}_x]} \tag{16}$$

because

$$\frac{\partial \frac{k}{k+x}}{\partial x} = -\frac{k}{(k+x)^2} \tag{17}$$

Table 2: Jacobian for general decomposition (add for each rate term)

	C_u	C_{di}	C_m	N_u	N_{di}	N_m	P_u	P_{di}	P_m
C_u	$-\frac{\partial R}{\partial \mathrm{C}_u}$	$-\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$-\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$-\frac{\partial R}{\partial \mathrm{P}_m}$
C_{di}	$d_i\frac{\partial R}{\partial \mathrm{C}_u}$	$d_i\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$d_i\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$d_i\frac{\partial R}{\partial \mathrm{P}_m}$
C_m	$(1-d_i)\frac{\partial R}{\partial \mathrm{C}_u}$	$(1-d_i)\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$(1-d_i)\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$(1-d_i)\frac{\partial R}{\partial \mathrm{N}_m}$
N_u	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_u}$	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$-\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{P}_m}$
N_{di}	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_u}$	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{P}_m}$
N_m	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_u}$	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}}]\right)\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\left(\frac{[\mathrm{N}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{N}_{di}]}{[\mathrm{C}_{di}}]\right)\frac{\partial R}{\partial \mathrm{P}_m}$
P_u	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_u}$	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$-\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]}\frac{\partial R}{\partial \mathrm{P}_m}$
P_{di}	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_u}$	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\frac{\partial R}{\partial \mathrm{P}_m}$
P_m	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_u}$	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}]}\right)\frac{\partial R}{\partial \mathrm{C}_{di}}$	0	0	0	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}}]\right)\frac{\partial R}{\partial \mathrm{N}_m}$	0	0	$\left(\frac{[\mathrm{P}_u]}{[\mathrm{C}_u]} - \frac{[\mathrm{P}_{di}]}{[\mathrm{C}_{di}}]\right)\frac{\partial R}{\partial \mathrm{P}_m}$

Table 3: Jacobian for general decomposition (add only once)

	C_u	C_{di}	C_m	N_u	N_{di}	N_m	P_u	P_{di}	P_m
C_u	0	0	0	0	0	0	0	0	0
C_{di}	0	0	0	0	0	0	0	0	0
C_m	0	0	0	0	0	0	0	0	0
N_u	$\frac{[N_u]}{[C_u]^2}R$	0	0	$-\frac{1}{[C_u]}R$	0	0	0	0	0
N_{di}	0	$-\frac{[N_{di}]}{[C_{di}]^2}R$	0	0	$\frac{1}{[C_{di}]}R$	0	0	0	0
N_m	$-\frac{[N_u]}{[C_u]^2}R$	$\frac{[N_{di}]}{[C_{di}]^2}R$	0	$\frac{1}{[C_u]}R$	$-\frac{1}{[C_{di}]}R$	0	0	0	0
P_u	$\frac{[P_u]}{[C_u]^2}R$	0	0	0	0	0	$-\frac{1}{[C_u]}R$	0	0
P_{di}	0	$-\frac{[P_{di}]}{[C_{di}]^2}R$	0	0	0	0	0	$\frac{1}{[C_{di}]}R$	0
P_m	$-\frac{[P_u]}{[C_u]^2}R$	$\frac{[P_{di}]}{[C_{di}]^2}R$	0	0	0	0	$\frac{1}{[C_u]}R$	$-\frac{1}{[C_{di}]}R$	0

2 Application Examples

2.1 Example 1. First Order

2.1.1 Input

```
IMMOBILE_SPECIES
  C
  SOM1
  Lit1
/
REACTION_SANDBOX
  CLM-CNP
    UPSTREAM
      CPOOL Lit1
    /
    DOWNSTREAM
      CPOOL SOM1 0.61
    /
   FIRSTORDER Lit1
   RATE_CONSTANT 0.7 1/d
  /
/
```

2.1.2 Results

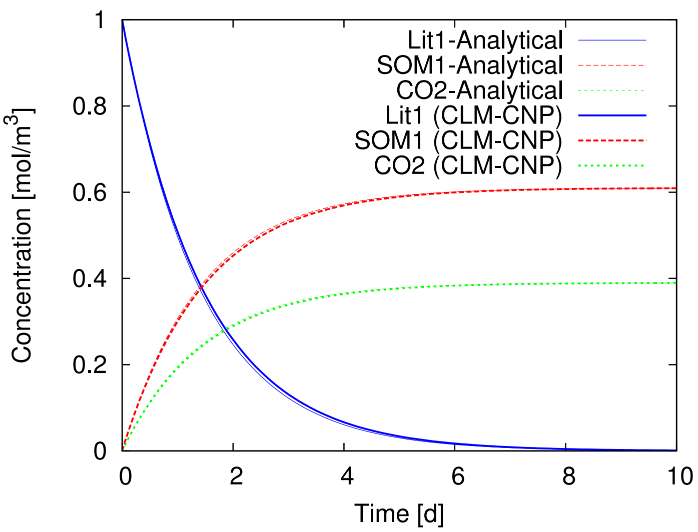

Figure 1: Demonstrating simple decomposition

2.2 Example 2. Add N

2.2.1 Input

```
    C
    N
    Lit1C
    Lit1N
    SOM1
  /
  REACTION_SANDBOX
    CLM-CNP
      UPSTREAM
        CPOOL Lit1C
        NPOOL Lit1N
      /
      DOWNSTREAM
        CPOOL SOM1 0.61
        CNRATIO 12.d0
      /
     FIRSTORDER Lit1C
     RATE_CONSTANT 0.7 1/d
    /
  /
```

2.2.2 Results

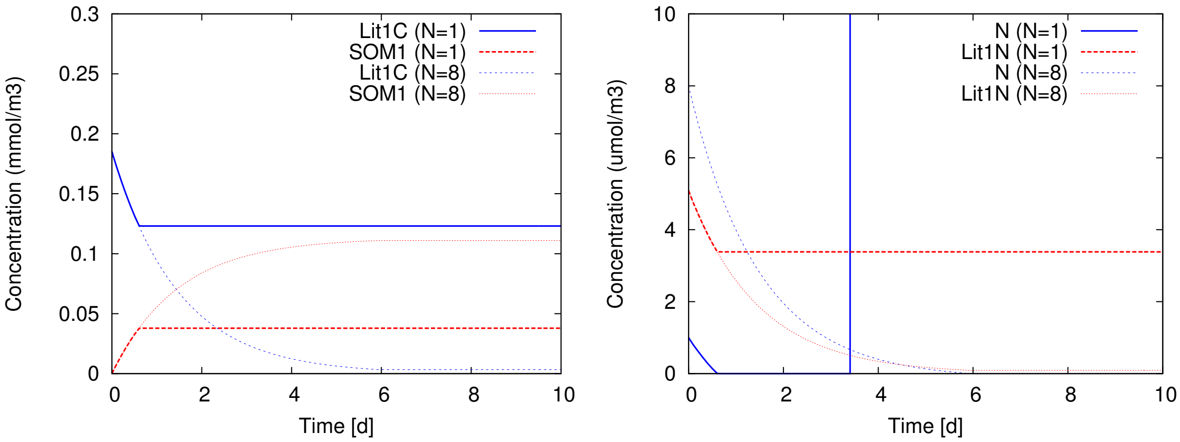

Figure 2: Add N

2.3 Example 3. Add P

2.3.1 Input

```
IMMOBILE_SPECIES
  C
  N
  Lit1C
  Lit1N
  SOM1
  P
  Lit1P
/
REACTION_SANDBOX
  CLM-CNP
    UPSTREAM
      CPOOL Lit1C
      NPOOL Lit1N
      PPOOL Lit1P
    /
    DOWNSTREAM
      CPOOL SOM1 0.61
      CNRATIO 12.d0
      CPRATIO 350.d0
    /
   FIRSTORDER Lit1C
   RATE_CONSTANT 0.7 1/d
  /
/
```

2.3.2 Results

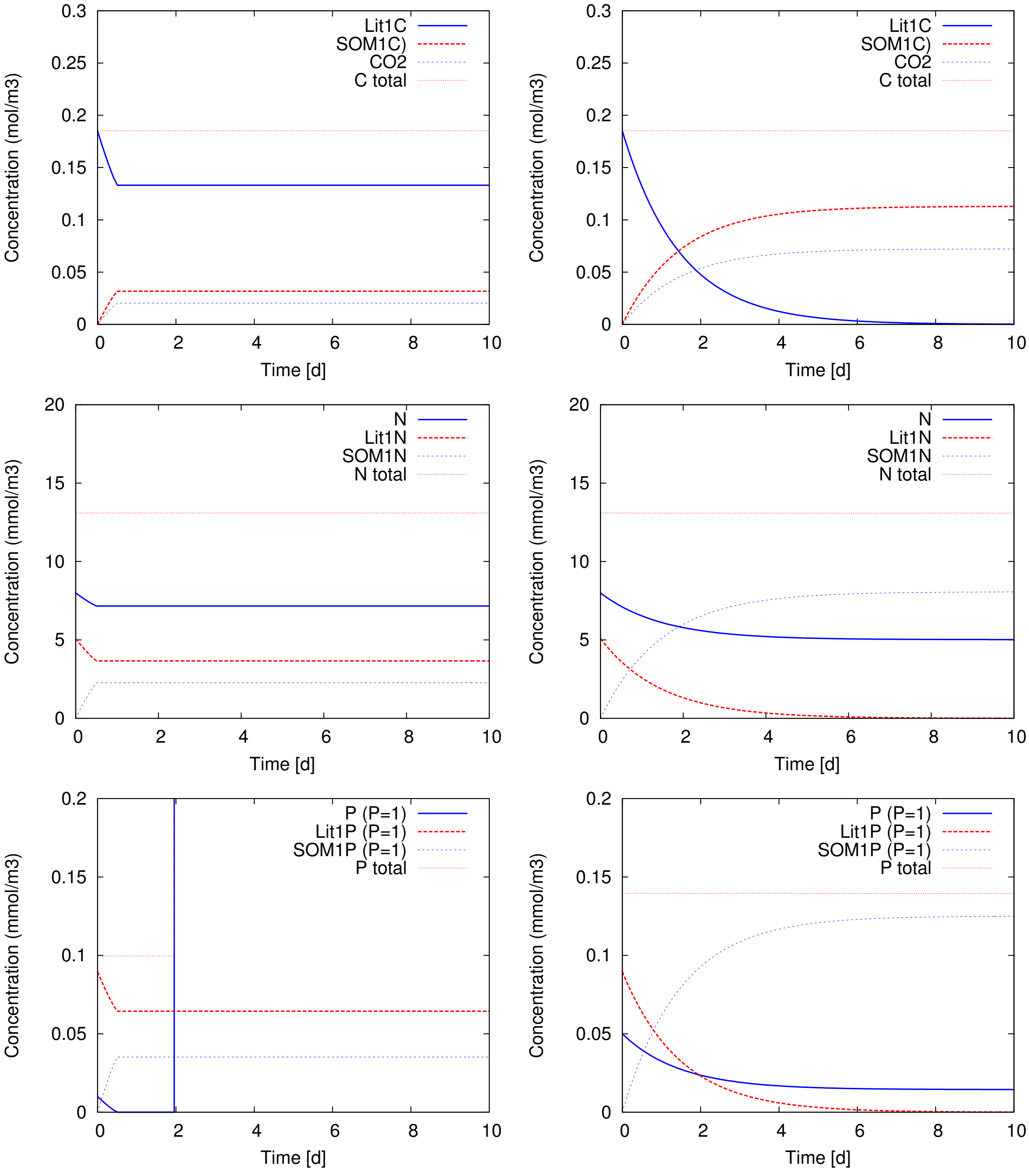

Figure 3: Add P

2.4 Example 4. Monod

2.4.1 Input

```
IMMOBILE_SPECIES
  C
  SOM1
  Lit1
  MBC
/
REACTION_SANDBOX
  CLM-CNP
    UPSTREAM
      CPOOL Lit1
    /
    DOWNSTREAM
      CPOOL SOM1 0.56
    /
    DOWNSTREAM
      CPOOL MBC  0.05
    /
   FIRSTORDER MBC
   MONOD Lit1 1.0d-4
   RATE_CONSTANT 7.0 1/d
  /
/
```

2.4.2 Results

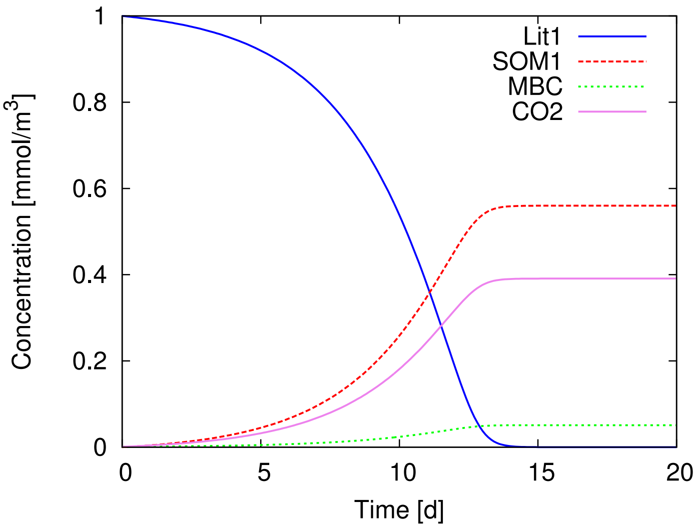

Figure 4: Add MBC and Use Monod

2.5 Example 5. Michaelis-Menten

2.5.1 Input

```
IMMOBILE_SPECIES
  C
  SOM1
  Lit1
  MBC
  Enzyme
/
REACTION_SANDBOX
  CLM-CNP
    UPSTREAM
      CPOOL Lit1
    /
    DOWNSTREAM
      CPOOL SOM1 0.56
    /
    DOWNSTREAM
      CPOOL MBC  0.04
    /
    DOWNSTREAM
      CPOOL Enzyme 0.01
    /
   FIRSTORDER Enzyme
   MONOD Lit1 1.0d-4
   RATE_CONSTANT 70.0 1/d
  /
/
```

2.5.2 Results

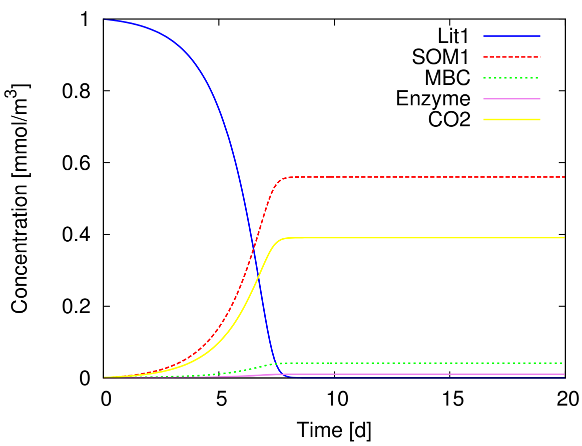

Figure 5: Add Enzyme and use Michaelis-Menten

2.6 Example 6. CLM-CN without N

2.6.1 Input

```
  IMMOBILE_SPECIES
    C
    Lit1
    Lit2
    Lit3
    SOM1
    SOM2
    SOM3
    SOM4
    SOMD
  /
  REACTION_SANDBOX
: Lit1 -> 0.61 SOM1 + 0.39 CO2
    CLM-CNP
      UPSTREAM
        CPOOL Lit1
      /
      DOWNSTREAM
        CPOOL SOM1 0.61
      /
     FIRSTORDER Lit1
     RATE_CONSTANT 0.7 1/d
    /
: Lit2 -> 0.45 SOM2 + 0.55 CO2
   CLM-CNP
     UPSTREAM
       CPOOL Lit2
     /
     DOWNSTREAM
       CPOOL SOM2 0.45
     /
    FIRSTORDER Lit2
    RATE_CONSTANT 0.07 1/d
   /
: Lit3 -> 0.71 SOM3 + 0.29 CO2
   CLM-CNP
     UPSTREAM
       CPOOL Lit3
     /
     DOWNSTREAM
       CPOOL SOM3 0.71
     /
    FIRSTORDER Lit3
```

```
    RATE_CONSTANT 0.014 1/d
   /
: SOM1 -> 0.72 SOM2 + 0.28 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM1
     /
     DOWNSTREAM
       CPOOL SOM2 0.72
     /
    FIRSTORDER SOM1
    RATE_CONSTANT 0.07 1/d
   /
: SOM2 -> 0.54 SOM3 + 0.46 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM2
     /
     DOWNSTREAM
       CPOOL SOM3 0.54
     /
    FIRSTORDER SOM2
    RATE_CONSTANT 0.014 1/d
   /
: SOM3 -> 0.45 SOM4 + 0.55 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM3
     /
     DOWNSTREAM
       CPOOL SOM4 0.45
     /
    FIRSTORDER SOM3
    RATE_CONSTANT 0.0014 1/d
   /
: SOM4 -> 0.39 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM4
     /
     DOWNSTREAM
       CPOOL SOMD 0.0d0
     /
    FIRSTORDER SOM4
    RATE_CONSTANT 0.0001 1/d
   /
```

/

2.6.2 Results

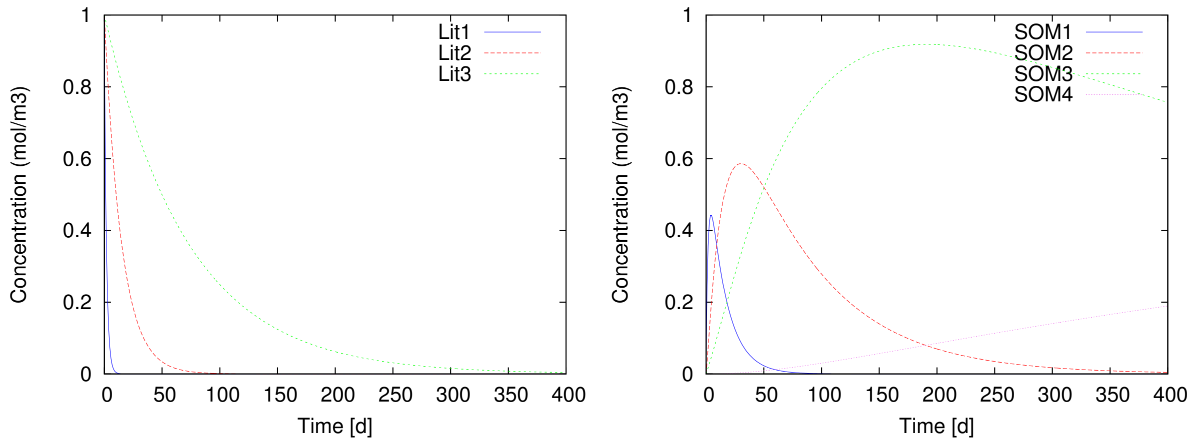

Figure 6: CLM-C

2.7 Example 7. CLM-CN

2.7.1 Input

```
  IMMOBILE_SPECIES
    C
    N
    Lit1C
    Lit1N
    Lit2C
    Lit2N
    Lit3C
    Lit3N
    SOM1
    SOM2
    SOM3
    SOM4
    SOMD
  /
  REACTION_SANDBOX
: Lit1 -> 0.61 SOM1 + 0.39 CO2
    CLM-CNP
      UPSTREAM
        CPOOL Lit1C
        NPOOL Lit1N
      /
      DOWNSTREAM
        CPOOL SOM1 0.61
        CNRATIO 12.d0
      /
     FIRSTORDER Lit1C
     RATE_CONSTANT 0.7 1/d
    /
: Lit2 -> 0.45 SOM2 + 0.55 CO2
   CLM-CNP
     UPSTREAM
       CPOOL Lit2C
       NPOOL Lit2N
     /
     DOWNSTREAM
       CPOOL SOM2 0.45
       CNRATIO 12.d0
     /
    FIRSTORDER Lit2C
    RATE_CONSTANT 0.07 1/d
   /
: Lit3 -> 0.71 SOM3 + 0.29 CO2
```

```
   CLM-CNP
     UPSTREAM
       CPOOL Lit3C
       NPOOL Lit3N
     /
     DOWNSTREAM
       CPOOL SOM3 0.71
       CNRATIO 10.d0
     /
    FIRSTORDER Lit3C
    RATE_CONSTANT 0.014 1/d
   /
: SOM1 -> 0.72 SOM2 + 0.28 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM1
       CNRATIO 12.d0
     /
     DOWNSTREAM
       CPOOL SOM2 0.72
       CNRATIO 12.d0
     /
    FIRSTORDER SOM1
    RATE_CONSTANT 0.07 1/d
   /
: SOM2 -> 0.54 SOM3 + 0.46 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM2
       CNRATIO 12.d0
     /
     DOWNSTREAM
       CPOOL SOM3 0.54
       CNRATIO 10.d0
     /
    FIRSTORDER SOM2
    RATE_CONSTANT 0.014 1/d
   /
: SOM3 -> 0.45 SOM4 + 0.55 CO2
   CLM-CNP
     UPSTREAM
       CPOOL SOM3
       CNRATIO 10.d0
     /
     DOWNSTREAM
       CPOOL SOM4 0.45
```

```
      CNRATIO 10.d0
    /
   FIRSTORDER SOM3
   RATE_CONSTANT 0.0014 1/d
  /
: SOM4 -> 0.39 CO2
  CLM-CNP
    UPSTREAM
      CPOOL SOM4
      CNRATIO 10.d0
    /
    DOWNSTREAM
      CPOOL SOMD 0.0d0
      CNRATIO 10.d0
    /
   FIRSTORDER SOM4
   RATE_CONSTANT 0.0001 1/d
  /
 /
```

2.7.2 Results

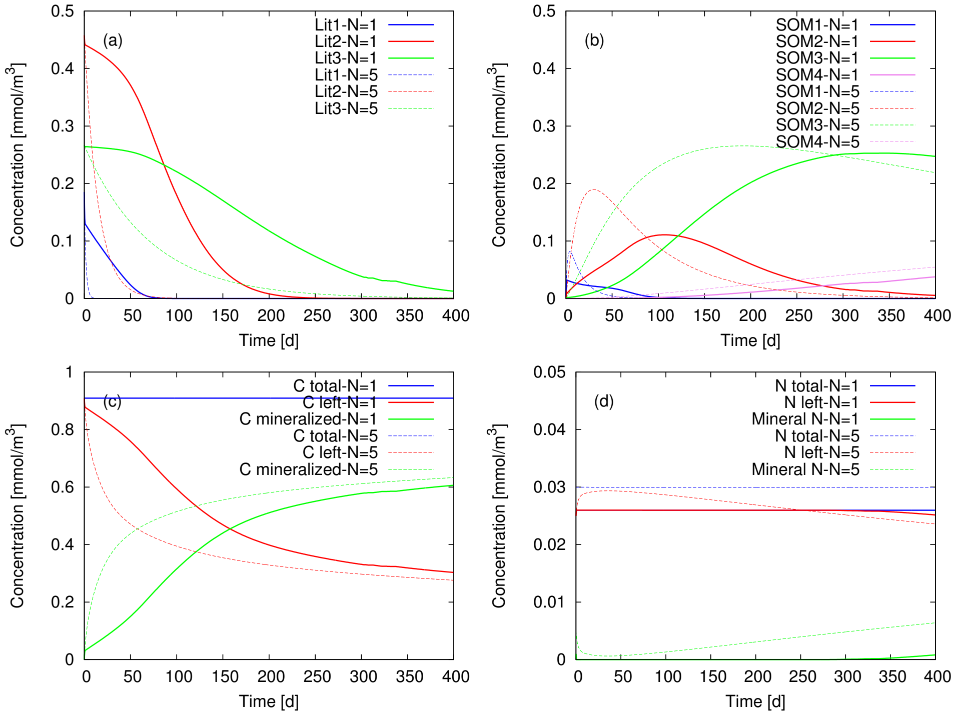

Figure 7: Adding P

2.8 Example 8. CLM-CNP

2.8.1 Input

```
  IMMOBILE_SPECIES
    C
    N
    Lit1C
    Lit1N
    Lit2C
    Lit2N
    Lit3C
    Lit3N
    SOM1
    SOM2
    SOM3
    SOM4
    SOMD
    P
    Lit1P
    Lit2P
    Lit3P
  /
  REACTION_SANDBOX
: Lit1 -> 0.61 SOM1 + 0.39 CO2
    CLM-CNP
      UPSTREAM
        CPOOL Lit1C
        NPOOL Lit1N
        PPOOL Lit1P
      /
      DOWNSTREAM
        CPOOL SOM1 0.61
        CNRATIO 12.d0
        CPRATIO 350.d0
      /
     FIRSTORDER Lit1C
     RATE_CONSTANT 0.7 1/d
    /
: Lit2 -> 0.45 SOM2 + 0.55 CO2
   CLM-CNP
     UPSTREAM
       CPOOL Lit2C
       NPOOL Lit2N
       PPOOL Lit2P
     /
     DOWNSTREAM
```

```
        CPOOL SOM2 0.45
        CNRATIO 12.d0
        CPRATIO 350.d0
      /
     FIRSTORDER Lit2C
     RATE_CONSTANT 0.07 1/d
    /
: Lit3 -> 0.71 SOM3 + 0.29 CO2
    CLM-CNP
      UPSTREAM
        CPOOL Lit3C
        NPOOL Lit3N
        PPOOL Lit3P
      /
      DOWNSTREAM
        CPOOL SOM3 0.71
        CNRATIO 10.d0
        CPRATIO 350.d0
      /
     FIRSTORDER Lit3C
     RATE_CONSTANT 0.014 1/d
    /
: SOM1 -> 0.72 SOM2 + 0.28 CO2
    CLM-CNP
      UPSTREAM
        CPOOL SOM1
        CNRATIO 12.d0
        CPRATIO 350.d0
      /
      DOWNSTREAM
        CPOOL SOM2 0.72
        CNRATIO 12.d0
        CPRATIO 350.d0
      /
     FIRSTORDER SOM1
     RATE_CONSTANT 0.07 1/d
    /
: SOM2 -> 0.54 SOM3 + 0.46 CO2
    CLM-CNP
      UPSTREAM
        CPOOL SOM2
        CNRATIO 12.d0
        CPRATIO 350.d0
      /
      DOWNSTREAM
        CPOOL SOM3 0.54
```

```
      CNRATIO 10.d0
      CPRATIO 350.d0
    /
   FIRSTORDER SOM2
   RATE_CONSTANT 0.014 1/d
  /
: SOM3 -> 0.45 SOM4 + 0.55 CO2
  CLM-CNP
    UPSTREAM
      CPOOL SOM3
      CNRATIO 10.d0
      CPRATIO 350.d0
    /
    DOWNSTREAM
      CPOOL SOM4 0.45
      CNRATIO 10.d0
      CPRATIO 350.d0
    /
   FIRSTORDER SOM3
   RATE_CONSTANT 0.0014 1/d
  /
: SOM4 -> 0.39 CO2
  CLM-CNP
    UPSTREAM
      CPOOL SOM4
      CNRATIO 10.d0
      CPRATIO 350.d0
    /
    DOWNSTREAM
      CPOOL SOMD 0.0d0
      CNRATIO 10.d0
      CPRATIO 350.d0
    /
   FIRSTORDER SOM4
   RATE_CONSTANT 0.0001 1/d
  /
 /
```

2.8.2 Results

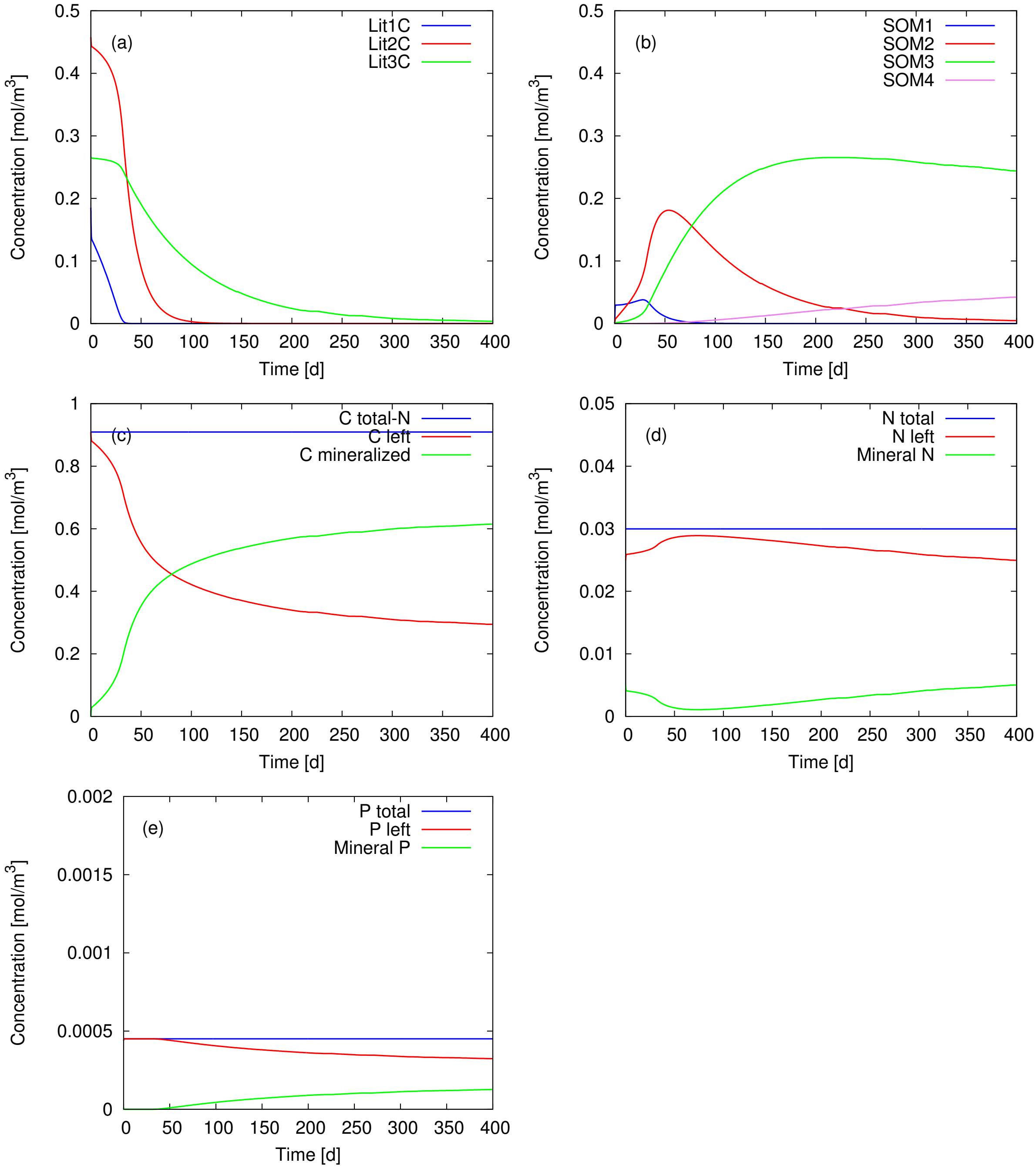

Figure 8: Adding P