

A mathematical model for bioremediation of hydrocarbon-contaminated soils

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Table S1. Stoichiometry of the main processes involved in hexadecane biodegradation

Reaction	Oxidation/Reduction couple
Biodegradation coupled to aerobic respiration $C_{16}H_{34} + 24.5 O_2 \rightarrow 16 HCO_3^- + H_2O + 16H^+$	O_2 / H_2O
Biodegradation coupled to denitrification $C_{16}H_{34} + 19.6 NO_3^- + 3.6 H^+ \rightarrow 16 HCO_3^- + 9.8 N_2 + 10.8 H_2O$	NO_3^- / N_2
Biodegradation coupled to Fe(III) reduction $C_{16}H_{34} + 98 Fe^{3+} + 48 H_2O \rightarrow 98 Fe^{2+} + 16 HCO_3^- + 114 H^+$	Fe^{3+} / Fe^{2+}
Biodegradation coupled to sulfate reduction $C_{16}H_{34} + 12.25 SO_4^{2-} + 8.5 H^+ \rightarrow 16 HCO_3^- + 12.25 H_2S + H_2O$	SO_4^{2-} / H_2S
Biodegradation coupled to methanogenesis $C_{16}H_{34} + 11.25 H_2O \rightarrow 3.75 HCO_3^- + 12.25 CH_4 + 3.75H^+$	HCO_3^- / CH_4

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Table S2. Stoichiometric (Petersen) and composition matrix for the bioremediation model

Component Process	C_C16H34	C_NO3	C_SO4	C_CH4	C_Fe2+	C_O2	X_aer	X_dnb	X_srb	X_irb	X_met	S_C16H34	S_NO3	S_SO4	S_Fe3+
1. Aerobic biodegradation	$-\frac{1}{113}$					$-\frac{24.5}{113}$	1								
2. Death of aerobic bacteria							-1								
3. Biodegradation coupled to denitrification	$-\frac{1}{113}$	$-\frac{19.6}{113}$						1							
4. Death of denitrifying microorganisms								-1							
5. Biodegradation coupled to iron(III) reduction	$-\frac{1}{113}$				$-\frac{98}{113}$					1					
6. Death of Fe(III)-reducing microorganisms										-1					
7. Biodegradation coupled to sulfate reduction	$-\frac{1}{113}$		$-\frac{12.25}{113}$						1						
8. Death of sulfate-reducing microorganisms									-1						
9. Biodegradation under methanogenic conditions	$-\frac{1}{113}$			$-\frac{12.25}{113}$							1				
10. Death of methanogenic microorganisms											-1				
11. Adsorption of hydrocarbon	$-\rho\left(\frac{1-\theta}{\theta}\right)$											1			
12. Adsorption of nitrate		$-\rho\left(\frac{1-\theta}{\theta}\right)$											1		
13. Adsorption of sulfate			$-\rho\left(\frac{1-\theta}{\theta}\right)$											1	
14. Re-oxidation of Fe ²⁺															1

Table S3. Values of model parameters and constants

Name	Description	Value	Unit	Reference
n_{TPH}	Exponential coefficient from Freundlich isotherm for hexadecane	0.6712	-	This study
n_{NO_3}	Exponential coefficient from Freundlich isotherm for nitrate	1.305	-	[1]
n_{SO_4}	Exponential coefficient from Freundlich isotherm for sulfate	1.312	-	[2]
K_{f,NO_3^-}	Adsorption constant for nitrate	0.01265	L/kg	[1]
$K_{f,TPH}$	Adsorption constant for hexadecane	0.00435	L/kg	This study
$K_{f,SO_4^{2-}}$	Adsorption constant for sulfate	0.01315	L/kg	[2]
$\beta_{X_{aer}}$	Temperature correction factor for aerobic microorganisms	0.04	-	[3]
$b_{X_{anae}}$	Temperature correction factor for anaerobic microorganisms	0.06	-	[3]
k	Relaxing constant	10 000	h ⁻¹	[4]
k_{FeOx}	Iron(II) oxidation constant into iron(III)	1000	d ⁻¹	This study
$k_{death,X_{aer},20}$	Death rate for aerobic microorganisms at 20 °C	0.002	d ⁻¹	[5]
$k_{death,X_{anae},20}$	Death rate for anaerobic microorganisms at 20 °C	0.002	d ⁻¹	[5]
$K_{s,TPH}$	Half saturation constant for the biodegradation of TPH	4.5	mg/L	[5]
$K_{s,Fe(OH)_3}$	Half saturation constant for iron	0.15	mg/L	This study
K_{s,NO_3^-}	Half saturation constant for nitrate	0.15	mg/L	[6]
K_{s,O_2}	Half saturation constant for oxygen	0.1	mg/L	[7]
$K_{s,SO_4^{2-}}$	Half saturation constant for sulfate	0.15	mg/L	This study
$u_{max,met,20}$	TPH biodegradation rate under methanogenic conditions at 20 °C	0.01367	d ⁻¹	[8]
$u_{max,Fe(III),20}$	TPH biodegradation rate in the presence of iron(III) at 20 °C	0.0199	d ⁻¹	[6]
$u_{max,den,20}$	TPH biodegradation rate in the presence of nitrate at 20 °C	0.114	d ⁻¹	This study
$u_{max,aer,20}$	TPH biodegradation rate in the presence of oxygen at 20 °C	0.587	d ⁻¹	This study
$u_{max,sulf,20}$	TPH biodegradation rate in the presence of sulfate at 20 °C	0.04	d ⁻¹	[6]
ρ	Soil density	1600	kg/m ³	[5]
θ	Soil porosity	0.5	-	[5]

Table S4. Values of absolute-relative sensitivity (Sens AR) of model parameters on TPH concentration in the liquid and solid phases (expressed as mg/L and g/kg, respectively)

Rank	C _{TPH}		S _{TPH}	
	Parameter	Sensitivity (mg/L)	Parameter	Sensitivity (g/kg)
1	n_{TPH}	79.07	$u_{max,met,20}$	1.305
2	$u_{max,met,20}$	67.64	n_{TPH}	1.004
3	$K_{f,TPH}$	15.73	θ	0.239
4	θ	11.49	$k_{death,X_{anae},20}$	0.215
5	$k_{death,X_{anae},20}$	11.21	ρ	0.211
6	$K_{s,TPH}$	10.61	$K_{s,TPH}$	0.200
7	ρ	10.13	$K_{f,TPH}$	0.188
8	n_{NO_3}	0.511	n_{NO_3}	0.016
9	$u_{max,den,20}$	0.319	$u_{max,den,20}$	0.0101
10	$u_{max,aer,20}$	0.305	$u_{max,sulf,20}$	0.0073
11	$k_{death,X_{aer},20}$	0.236	$k_{death,X_{aer},20}$	0.0047
12	$u_{max,sulf,20}$	0.228	$u_{max,aer,20}$	0.0047
13	$n_{SO_4^{2-}}$	0.118	$n_{SO_4^{2-}}$	0.0036
14	K_{f,NO_3^-}	0.110	K_{f,NO_3^-}	0.0035
15	$K_{f,SO_4^{2-}}$	0.061	$K_{f,SO_4^{2-}}$	0.0018
16	K_{s,O_2}	0.052	K_{s,O_2}	0.0009
17	$u_{max,Fe(III),20}$	0.033	$u_{max,Fe(III),20}$	0.0007
18	$K_{s,SO_4^{2-}}$	0.004	$K_{s,SO_4^{2-}}$	0.0001
19	k_{FeOx}	0.002	k_{FeOx}	0.0000
20	$K_{s,Fe(OH)}$	0.002	$K_{s,Fe(OH)}$	0.0000
21	K_{s,NO_3^-}	0.002	K_{s,NO_3^-}	0.0000
22	k	0.001	k	0.0000
23	$\beta_{X_{anae}}$	0.000	$\beta_{X_{aer}}$	0.0000
24	$\beta_{X_{aer}}$	0.000	$\beta_{X_{anae}}$	0.0000

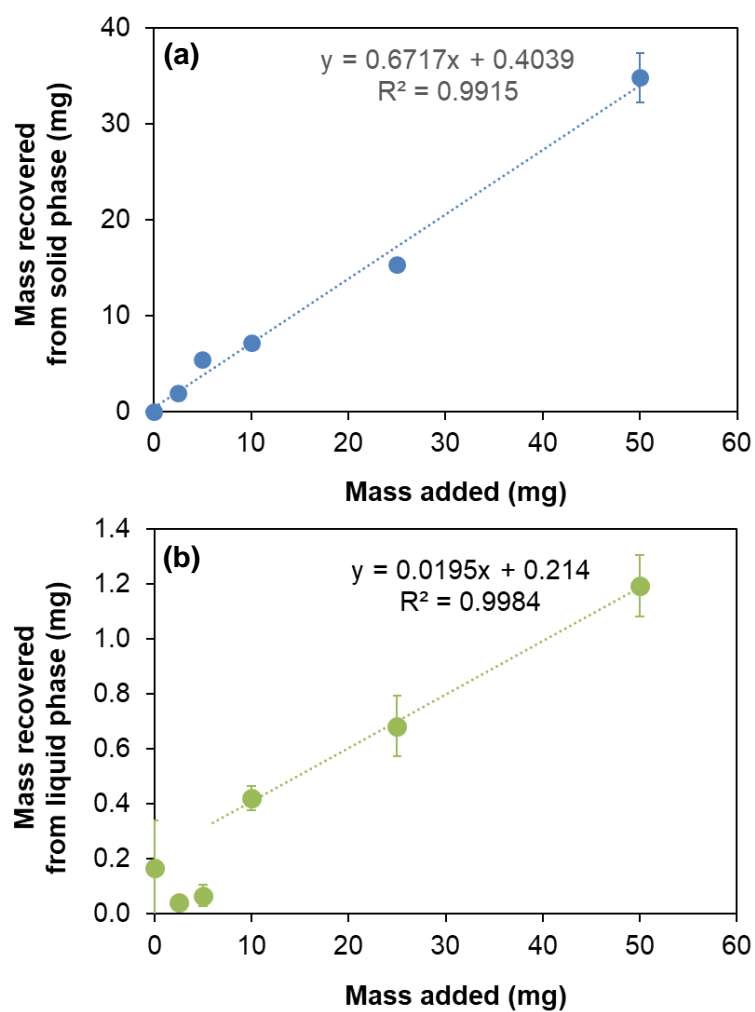


Figure S1. Hexadecane mass recovered from solid (a) and liquid (b) phases, relatively to the mass added in the solid-liquid partition experiments. The results presented are the averages and standard deviations for quadruplicate assays.

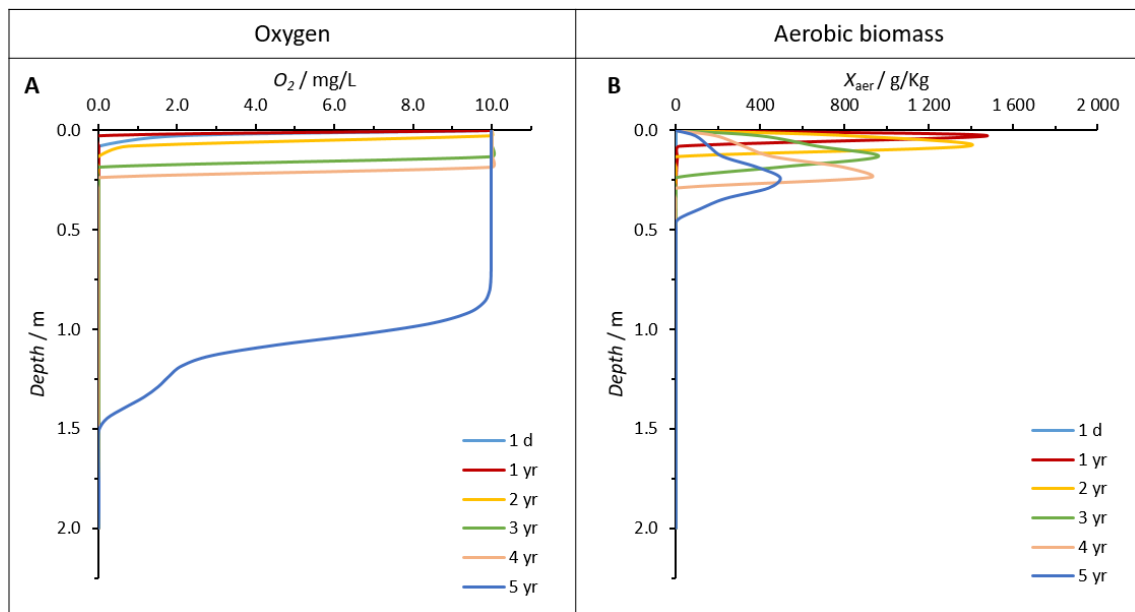


Figure S2. Variation of dissolved oxygen (A) and aerobic biomass (B) concentrations in depth.

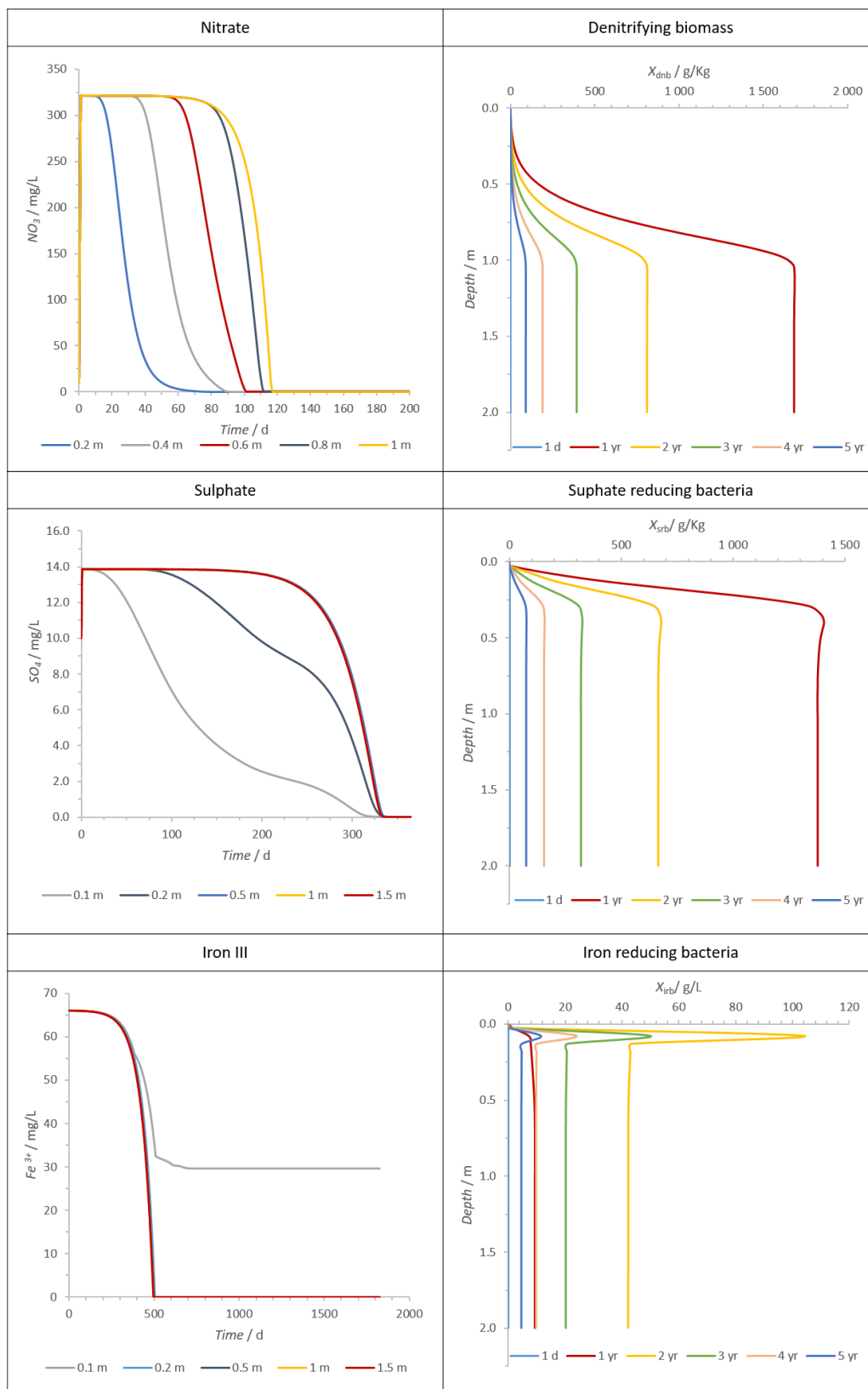


Figure S3. Variation of nitrate, sulfate and Fe(III) over time, and denitrifying, sulfate reducing and iron reducing bacteria in depth.

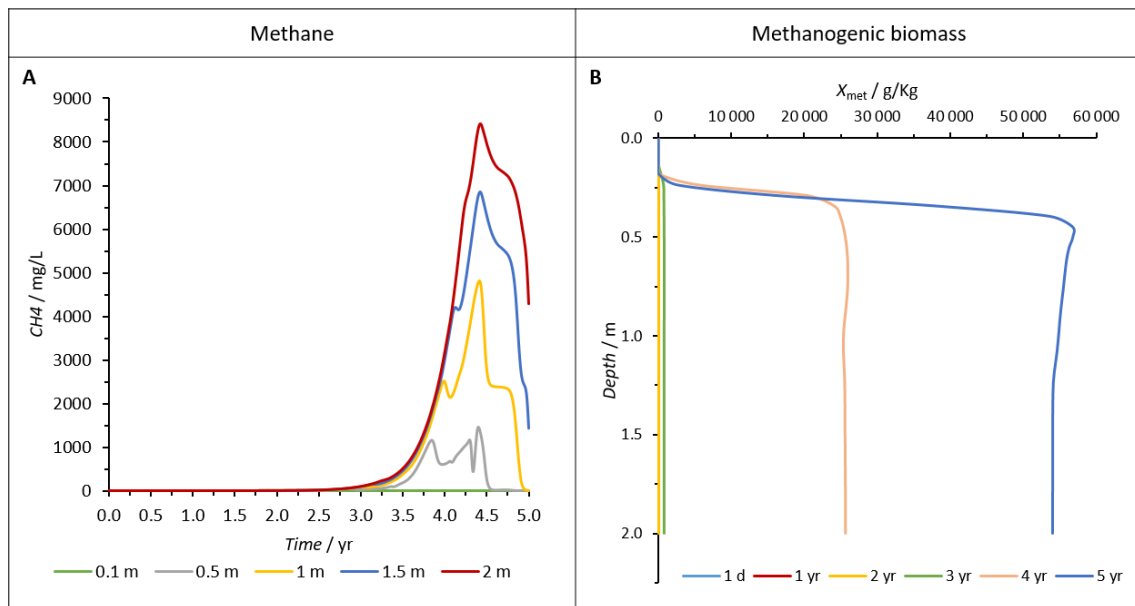


Figure S4. Variation of methane concentration over time (A), and of methanogenic biomass concentration in depth (B).

References

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Annex B: AQUASIM system definition

AQUASIM Version 2.1e (win/mfc) - Listing of System Definition

Date of listing: 08/30/2022

Variables

A: Description: Cross sectional area

 Type: Formula Variable

 Unit: m^2

 Expression: 1

alfa_C16: Description: Exponential coefficient from Freund

 lich isotherm for hexadecane

 Type: Constant Variable

 Unit:

 Value: 1.4898043

 Standard Deviation: 0.14898

 Minimum: 1.1918

 Maximum: 1.78776

 Sensitivity Analysis: active

 Parameter Estimation: inactive

alfa_NO3: Description: Exponential coefficient from Freund

 lich isotherm for nitrate

Type: Constant Variable

Unit:

Value: 0.7663

Standard Deviation: 0.07663

Minimum: 0.613

Maximum: 0.92

Sensitivity Analysis: active

Parameter Estimation: inactive

alfa_SO4: Description: Exponential coefficient from Freund

lich isotherm for sulfate

Type: Constant Variable

Unit:

Value: 0.7623

Standard Deviation: 0.07623

Minimum: 0.61

Maximum: 0.915

Sensitivity Analysis: active

Parameter Estimation: inactive

beta_Xaer: Description: Temperature correction factor for a

erobic microorganisms

Type: Constant Variable

Unit:

Value: 0.04

Standard Deviation: 0.004

Minimum: 0.032

Maximum: 0.048

Sensitivity Analysis: active

Parameter Estimation: inactive

beta_Xanaer: Description: Temperature correction factor for a
naerobic microorganisms

Type: Constant Variable

Unit:

Value: 0.06

Standard Deviation: 0.006

Minimum: 0.048

Maximum: 0.072

Sensitivity Analysis: active

Parameter Estimation: inactive

C_CH4: Description: Methane concentration in the liquid
phase

Type: Dyn. Volume State Var.

Unit: mg/L

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

C_critic: Description: Critic concentration

Type: Constant Variable

Unit: mg/m³

Value: 0.001

Standard Deviation: 0.0001

Minimum: 0.0008

Maximum: 0.0012

Sensitivity Analysis: active

Parameter Estimation: inactive

C_Fell: Description: Iron(II) concentration in the liquid phase

Type: Dyn. Volume State Var.

Unit: mg/L

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

C_ini_Fell: Description: Initial concentration of Fell

Type: Formula Variable

Unit: mg/L

Expression: 0

C_ini_NO3: Description: Initial concentration of NO3

Type: Formula Variable

Unit: mg/L

Expression: 10

C_ini_SO4: Description: Initial concentration of SO4

Type: Formula Variable

Unit: mg/L

Expression: 10

C_in_NO3: Description: input concentration of NO3

Type: Formula Variable

Unit: mg/L

Expression: 0

C_in_SO4: Description: input concentration of SO4

Type: Formula Variable

Unit: mg/L

Expression: 0

C_in_TPH: Description: input concentration of TPH

Type: Real List Variable

Unit: mg/L

Argument: t

Standard Deviations: global

Rel. Stand. Deviat.: 0

Abs. Stand. Deviat.: 1

Minimum: 0

Maximum: 1e+009

Interpolation Method: linear interpolation

Sensitivity Analysis: inactive

Real Data Pairs (7 pairs):

0 0

1 0

1.1 0

2.1 0

2.2 0

365 0
3650 0

C_NO3: Description: Nitrate concentration in the liquid
phase
Type: Dyn. Volume State Var.
Unit: mg/L
Relative Accuracy: 1e-006
Absolute Accuracy: 1e-006

C_O2: Description: Dissolved oxygen concentration
Type: Dyn. Volume State Var.
Unit: mg/L
Relative Accuracy: 1e-006
Absolute Accuracy: 1e-006

C_O2_in: Description: input dissolved oxygen concentration
n
Type: Formula Variable
Unit: mg/L
Expression: 10

C_SO4: Description: Sulfate concentration in the liquid
phase
Type: Dyn. Volume State Var.
Unit: mg/L
Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

C_TPH: Description: Total petroleum hydrocarbon concent

ration in the liquid phase

Type: Dyn. Volume State Var.

Unit:

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

C_TPH_ini: Description: initial soluble concentration of TP

H

Type: Formula Variable

Unit: mg/L

Expression: 0

k: Description: Relaxation time constant

Type: Constant Variable

Unit: 1/h

Value: 10000

Standard Deviation: 1000

Minimum: 8000

Maximum: 12000

Sensitivity Analysis: active

Parameter Estimation: inactive

Kc_Fe: Description: Half saturation constant for iron

Type: Constant Variable

Unit: mg/L

Value: 0.15

Standard Deviation: 0.015

Minimum: 0.12

Maximum: 0.18

Sensitivity Analysis: active

Parameter Estimation: inactive

Kc_NO3: Description: Half saturation constant for nitrat

e

Type: Constant Variable

Unit: mg/L

Value: 0.15

Standard Deviation: 0.015

Minimum: 0.12

Maximum: 0.18

Sensitivity Analysis: active

Parameter Estimation: inactive

Kc_O2: Description: Half saturation constant for oxygen

Type: Constant Variable

Unit: mg/L

Value: 0.1

Standard Deviation: 0.01

Minimum: 0.08

Maximum: 0.12

Sensitivity Analysis: active

Parameter Estimation: inactive

Kc_SO4: Description: Half saturation constant for sulfat

e

Type: Constant Variable

Unit: mg/L

Value: 0.15

Standard Deviation: 0.015

Minimum: 0.12

Maximum: 0.18

Sensitivity Analysis: active

Parameter Estimation: inactive

Kc_TPH: Description: Half saturation constant for the bi

odegradation of TPH

Type: Constant Variable

Unit: mg/L

Value: 4.5

Standard Deviation: 0.031

Minimum: 0.248

Maximum: 10

Sensitivity Analysis: active

Parameter Estimation: inactive

k_death_Xaer: Description: Death rate for aerobic microorganis

ms

Type: Formula Variable

Unit: d-1

Expression: $k_death_Xaer_20 * \exp(\beta_Xaer * (T - 20))$

k_death_Xaer_20:

Description: Death rate for aerobic microorganism
at 20 °C

Type: Constant Variable

Unit: d-1

Value: 0.002

Standard Deviation: 0.0002

Minimum: 0.0016

Maximum: 0.04

Sensitivity Analysis: active

Parameter Estimation: inactive

k_death_Xanaer: Description: Death rate for anaerobic microorganisms

Type: Formula Variable

Unit: d-1

Expression: $k_death_Xanaer_20 * \exp(\beta_Xanaer * (T - 20))$

k_death_Xanaer_20:

Description: Death rate for anaerobic microorganisms
at 20 °C

Type: Constant Variable

Unit: d-1
Value: 0.002
Standard Deviation: 0.0002
Minimum: 0.0016
Maximum: 0.04
Sensitivity Analysis: active
Parameter Estimation: inactive

k_FeOx: Description: Iron(II) oxidation constant into iron(III)

Type: Constant Variable
Unit: d-1
Value: 1000
Standard Deviation: 100
Minimum: 800
Maximum: 1200
Sensitivity Analysis: active
Parameter Estimation: inactive

k_F_C16: Description: Adsorption constant for hexadecane

Type: Constant Variable
Unit:
Value: 0.00435
Standard Deviation: 0.000435
Minimum: 0.003484
Maximum: 0.005226
Sensitivity Analysis: active

Parameter Estimation: inactive

k_F_NO3: Description: Adsorption constant for nitrate

Type: Constant Variable

Unit:

Value: 0.001265

Standard Deviation: 0.000127

Minimum: 0.001

Maximum: 0.002

Sensitivity Analysis: active

Parameter Estimation: inactive

k_F_SO4: Description: Adsorption constant for sulfate

Type: Constant Variable

Unit:

Value: 0.01315

Standard Deviation: 0.001315

Minimum: 0.011

Maximum: 0.016

Sensitivity Analysis: active

Parameter Estimation: inactive

Q: Description: Water flow into the column

Type: Program Variable

Unit: m3/d

Reference to: Discharge

Qin: Description: Water flow into the column

Type: Formula Variable

Unit: m3/d

Expression: 0.00375

Qin_t: Description: Water flow into the column

Type: Real List Variable

Unit: m3/d

Argument: t

Standard Deviations: global

Rel. Stand. Deviat.: 0

Abs. Stand. Deviat.: 1

Minimum: 0

Maximum: 1e+009

Interpolation Method: linear interpolation

Sensitivity Analysis: inactive

Real Data Pairs (140 pairs):

0	0.005533333
30	0.005533333
60	0.005533333
90	0.005233333
120	0.003966667
.	.
.	.
3555	0.000766667
3585	0.0022
3615	0.0044

3645 0.005366667

3650 0.005366667

Rho_S: Description: soil density

Type: Constant Variable

Unit: kg/m³

Value: 1600

Standard Deviation: 160

Minimum: 1280

Maximum: 1920

Sensitivity Analysis: active

Parameter Estimation: inactive

Seq_freundlick_C16H34:

Description: Freundlick isotherm

Type: Formula Variable

Unit: mg/kg

Expression: if C_TPH>C_critic then k_F_C16*C_T
PH^{alfa_C16} else k_F_C16*C_critic^a
lfa_C16*C_TPH/C_critic endif

Seq_freundlick_NO3:

Description: Freundlick isotherm

Type: Formula Variable

Unit: mg/kg

Expression: if C_NO3>C_critic then k_F_NO3*C_N
O3^{alfa_NO3} else k_F_NO3*C_critic^a

lfa_NO3*C_NO3/C_critic endif

Seq_freundlick_SO4:

Description: Freundlick isotherm

Type: Formula Variable

Unit: mg/kg

Expression: if C_SO4>C_critic then k_F_SO4*C_S
O4^alfa_SO4 else k_F_SO4*C_critic^a
lfa_SO4*C_SO4/C_critic endif

S_FeIII: Description: Concentration of amorphous iron

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

S_FeIII_ini: Description: initial concentration of amorphous
iron

Type: Formula Variable

Unit: g/kg

Expression: 66

S_NO3: Description: Nitrate concentration in the solid
phase

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

S_NO3_ini: Description: initial Nitrate concentration in the solid phase

Type: Formula Variable

Unit: g/kg

Expression: 0.3

S_SO4: Description: Sulfate concentration in the solid phase

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

S_SO4_ini: Description: initial Sulfate concentration in the solid phase

Type: Formula Variable

Unit: g/kg

Expression: 0.1

S_TPH: Description: Total petroleum hydrocarbon concentration in the solid phase

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

S_TPH_ini: Description: initial adsorbed concentration TPH

Type: Formula Variable

Unit: g/kg

Expression: 0.6

T: Description: Soil temperature

Type: Formula Variable

Unit: degC

Expression: 20

t: Description: Time

Type: Program Variable

Unit: d

Reference to: Time

theta: Description: soil porosity

Type: Constant Variable

Unit:

Value: 0.5

Standard Deviation: 0.05

Minimum: 0.4

Maximum: 0.6

Sensitivity Analysis: active

Parameter Estimation: inactive

umax_CH4: Description: TPH biodegradation rate under methanogenic conditions

Type: Formula Variable

Unit:

Expression: $umax_CH4_20 * \exp(\beta_{Xanaer} * (T - 20))$

umax_CH4_20: Description: TPH biodegradation rate under methanogenic conditions at 20 °C

Type: Constant Variable

Unit:

Value: 0.01367

Standard Deviation: 0.001367

Minimum: 0.010936

Maximum: 0.016404

Sensitivity Analysis: active

Parameter Estimation: inactive

umax_FeIII: Description: TPH biodegradation rate in the presence of iron(III)

Type: Formula Variable

Unit: d⁻¹

Expression: $umax_FeIII_20 * \exp(\beta_{Xanaer} * (T - 20))$

umax_FeIII_20: Description: TPH biodegradation rate in the presence of iron(III) at 20 °C

Type: Constant Variable

Unit:

Value: 0.0199

Standard Deviation: 0.00199

Minimum: 0.01791

Maximum: 0.02189

Sensitivity Analysis: active

Parameter Estimation: inactive

umax_NO3: Description: TPH biodegradation rate in the presence of nitrate

Type: Formula Variable

Unit: d-1

Expression: $umax_NO3_20 * \exp(\beta_{Xanaer} * (T - 20))$

umax_NO3_20: Description: TPH biodegradation rate in the presence of nitrate at 20 C

Type: Constant Variable

Unit: d-1

Value: 0.114

Standard Deviation: 0.0114

Minimum: 0.0912

Maximum: 0.1368

Sensitivity Analysis: active

Parameter Estimation: inactive

umax_O2: Description: TPH biodegradation rate in the presence of oxygen

Type: Formula Variable

Unit: d-1

Expression: $umax_O2_20 * \exp(\beta_{Xaer} * (T - 20))$

umax_O2_20: Description: TPH biodegradation rate in the pres

ence of oxygen at 20 °C

Type: Constant Variable

Unit: d-1

Value: 0.587

Standard Deviation: 0.0587

Minimum: 0.4696

Maximum: 0.7044

Sensitivity Analysis: active

Parameter Estimation: inactive

umax_SO4: Description: TPH biodegradation rate in the pres

ence of sulfate

Type: Formula Variable

Unit: d-1

Expression: $umax_SO4_20 * \exp(\beta_{Xanaer} * (T - 20))$

umax_SO4_20: Description: TPH biodegradation rate in the pres

ence of sulfate at 20 °C

Type: Constant Variable

Unit: d-1

Value: 0.04

Standard Deviation: 0.005

Minimum: 0.03

Maximum: 0.05

Sensitivity Analysis: active

Parameter Estimation: inactive

X_aer: Description: Concentration of aerobic microorgan
isms
Type: Dyn. Surface State Var.
Unit: g/kg
Relative Accuracy: 1e-006
Absolute Accuracy: 1e-006

X_aer_ini: Description: initial concentration of aerobic mi
croorganisms
Type: Formula Variable
Unit: g/kg
Expression: 0.08

X_anaer_ini: Description: initial concentration of anaerobic
microorganisms
Type: Formula Variable
Unit: g/kg
Expression: 0.04

X_den: Description: Concentration of denitrifying micro
organisms
Type: Dyn. Surface State Var.
Unit: g/kg
Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

X_irb: Description: Concentration of iron reducing micr

oorganisms

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

X_met: Description: Concentration of methanogenic micro

organisms

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

X_met_ini: Description: initial concentration of methanogen

ic microorganisms

Type: Formula Variable

Unit: g/kg

Expression: 0.02

X_srb: Description: Concentration of sulfate reducing m

icroorganisms

Type: Dyn. Surface State Var.

Unit: g/kg

Relative Accuracy: 1e-006

Absolute Accuracy: 1e-006

Z: Description: column depth

 Type: Program Variable

 Unit: m

 Reference to: Space Coordinate Z

Processes

adsorption_C16H34:

 Description: adsorption isothermic for hexadecane

 Type: Dynamic Process

 Rate: $k*(Seq_freundlick_C16H34-S_TPH)$

 Stoichiometry:

 Variable : Stoichiometric Coefficient

 C_TPH : $-Rho_S*(1-theta)/theta$

 S_TPH : 1

adsorption_NO3:Description: Isothermic adsorption for nitrate

 Type: Dynamic Process

 Rate: $k*(Seq_freundlick_NO3-S_NO3)$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_NO3 : $-\text{Rho_S} \cdot (1 - \theta) / \theta$

S_NO3 : 1

adsorption_SO4: Description: Isothermic adsorption for sulfate

Type: Dynamic Process

Rate: $k \cdot (\text{Seq_freundlick_SO4} - S_{\text{SO4}})$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_SO4 : $-\text{Rho_S} \cdot (1 - \theta) / \theta$

S_SO4 : 1

aerobic_degradation:

Description: Degradation of TPH in the presence
of O2

Type: Dynamic Process

Rate: $u_{\text{max_O2}} \cdot (C_{\text{TPH}} / (K_{\text{c_TPH}} + C_{\text{TPH}})) \cdot (C_{\text{O2}} / (K_{\text{c_O2}} + C_{\text{O2}})) \cdot X_{\text{aer}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_TPH : -1/113

C_O2 : -24.5/113

X_aer : 1

death_Xaer: Description: death of aerobic biomass

Type: Dynamic Process

Rate: $k_{\text{death_Xaer}} \cdot X_{\text{aer}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

X_{aer} : -1

death_Xden: Description: death of denitrifiers

Type: Dynamic Process

Rate: $k_{\text{death_Xanaer}} \cdot X_{\text{den}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

X_{den} : -1

death_Xirb: Description: death of iron reducers

Type: Dynamic Process

Rate: $k_{\text{death_Xanaer}} \cdot X_{\text{irb}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

X_{irb} : -1

death_Xmet: Description: death of methanogens

Type: Dynamic Process

Rate: $k_{\text{death_Xanaer}} \cdot X_{\text{met}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

X_{met} : -1

death_Xsrb: Description: death of sulfate reducers

Type: Dynamic Process

Rate: $k_{\text{death_Xanaer}} \cdot X_{\text{srb}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

$X_{\text{srb}} : -1$

denitrification:

Description: Degradation of TPH in the presence of NO₃

Type: Dynamic Process

Rate: $u_{\text{max_NO3}} \cdot (C_{\text{TPH}} / (K_{\text{c_TPH}} + C_{\text{TPH}})) \cdot (K_{\text{c_O2}} / (K_{\text{c_O2}} + C_{\text{O2}})) \cdot (C_{\text{NO3}} / (K_{\text{c_NO3}} + C_{\text{NO3}})) \cdot X_{\text{den}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

$C_{\text{TPH}} : -1/113$

$C_{\text{NO3}} : -19.6/113$

$X_{\text{den}} : 1$

iron_reduction:Description: Degradation of TPH in the presence of Fe(III)

Type: Dynamic Process

Rate: $u_{\text{max_FeIII}} \cdot (C_{\text{TPH}} / (K_{\text{c_TPH}} + C_{\text{TPH}})) \cdot (K_{\text{c_O2}} / (K_{\text{c_O2}} + C_{\text{O2}})) \cdot (S_{\text{FeIII}} / (K_{\text{c_Fe}} + S_{\text{FeIII}})) \cdot X_{\text{irb}}$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_TPH : -1/113

S_FeIII : -98/113

X_irb : 1

C_FeII : 98/113

methanogenesis:Description: conversion of TPH to methane

Type: Dynamic Process

Rate: $u_{\max_CH4} * (C_TPH / (Kc_TPH + C_TPH)) * (Kc_O2 / (Kc_O2 + C_O2)) * X_met$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_TPH : -1/113

C_CH4 : 12.25/113

X_met : 1

r_FeOx: Description:

Type: Dynamic Process

Rate: $k_FeOx * C_FeII * C_O2$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_FeII : -1

S_FeIII : 1

sulfate_reduction:

Description: Degradation of TPH in the presence
of SO4

Type: Dynamic Process

Rate:
$$\text{umax_SO4} * (\text{C_TPH} / (\text{Kc_TPH} + \text{C_TPH})) * (\text{Kc_O2} / (\text{Kc_O2} + \text{C_O2})) * (\text{C_SO4} / (\text{Kc_SO4} + \text{C_SO4})) * \text{X_srb}$$

Stoichiometry:

Variable : Stoichiometric Coefficient

C_TPH : -1/113

C_SO4 : -12.25/113

X_srb : 1

Compartments

soil_column: Description:

Type: Soil Column Compartment

Compartment Index: 0

Active Variables: C_TPH, C_FeII, C_NO3, C_O2, C_SO4,

S_TPH, S_NO3, S_SO4, X_aer, X_den,

S_FeIII, C_CH4, X_irb, X_met, X_srb

Active Processes: adsorption_NO3, adsorption_SO4, dea

th_Xaer, death_Xden, death_Xirb, de

ath_Xmet, death_Xsrb, r_FeOx, adsor

ption_C16H34, aerobic_degradation,

denitrification, iron_reduction, me

thanogenesis, sulfate_reduction

Initial Conditions:

Variable(Zone) : Initial Condition

S_TPH(Advective Zone) : S_TPH_ini

S_NO3(Advective Zone) : S_NO3_ini

S_SO4(Advective Zone) : S_SO4_ini

X_aer(Advective Zone) : X_aer_ini

X_irb(Advective Zone) : X_anaer_ini

X_met(Advective Zone) : X_met_ini

X_srb(Advective Zone) : X_anaer_ini

X_den(Advective Zone) : X_anaer_ini

C_TPH(Advective Zone) : C_TPH_ini

C_NO3(Advective Zone) : C_ini_NO3

C_SO4(Advective Zone) : C_ini_SO4

C_FeII(Advective Zone) : C_ini_FeII

S_FeIII(Advective Zone) : S_FeIII_ini

Q(Advective Zone) : Qin

Inflow: Qin_t

Loadings:

Variable : Loading

C_TPH : C_in_TPH*Qin_t

C_O2 : C_O2_in*Qin_t

C_NO3 : C_in_NO3*Qin_t

C_SO4 : C_in_SO4*Qin_t

Lateral Inflow: 0

Start Coordinate: 0

End Coordinate: 2

Cross Section: A

Adv. Vol. Fract.: theta

Parallel Zones:

Num. of Grid Pts: 40 (high resolution)

Accuracies:

Rel. Acc. Q: 0.0001

Abs. Acc. Q: 1e-006

Rel. Acc. D: 1e-006

Abs. Acc. D: 1e-006

Definitions of Calculations

calc0: Description:

Calculation Number: 0

Initial Time: 0

Initial State: given, made consistent

Step Size: 1

Num. Steps: 1825

Status: active for simulation

active for sensitivity analysis

Plot Definitions

C_CH4: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_CH4 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_CH4 [0,soil_column,Advective Zone,1]

Value : C_CH4 [0,soil_column,Advective Zone,0.1]

Value : C_CH4 [0,soil_column,Advective Zone,2]

Value : C_CH4 [0,soil_column,Advective Zone,0.5]

Value : C_CH4 [0,soil_column,Advective Zone,1.5]

C_CH4_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_CH4 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_CH4 [0,soil_column,Advective Zone,1]

Value : C_CH4 [0,soil_column,Advective Zone,365]

Value : C_CH4 [0,soil_column,Advective Zone,730]

Value : C_CH4 [0,soil_column,Advective Zone,1095]

Value : C_CH4 [0,soil_column,Advective Zone,1460]

Value : C_CH4 [0,soil_column,Advective Zone,1825]

Value : C_CH4 [0,soil_column,Advective Zone,2190]

Value : C_CH4 [0,soil_column,Advective Zone,2555]

Value : C_CH4 [0,soil_column,Advective Zone,2920]

Value : C_CH4 [0,soil_column,Advective Zone,3285]

Value : C_CH4 [0,soil_column,Advective Zone,3650]

C_Fell: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_Fell / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_Fell [0,soil_column,Advective Zone,1]

Value : C_Fell [0,soil_column,Advective Zone,0.1]

Value : C_Fell [0,soil_column,Advective Zone,2]

C_Fell_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_FeII / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_FeII [0,soil_column,Advective Zone,1]

Value : C_FeII [0,soil_column,Advective Zone,365]

Value : C_FeII [0,soil_column,Advective Zone,730]

Value : C_FeII [0,soil_column,Advective Zone,1095]

Value : C_FeII [0,soil_column,Advective Zone,1460]

Value : C_FeII [0,soil_column,Advective Zone,1825]

Value : C_FeII [0,soil_column,Advective Zone,2190]

Value : C_FeII [0,soil_column,Advective Zone,2555]

Value : C_FeII [0,soil_column,Advective Zone,2920]

Value : C_FeII [0,soil_column,Advective Zone,3285]

Value : C_FeII [0,soil_column,Advective Zone,3650]

C_NO3: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_NO3 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_NO3 [0,soil_column,Advective Zone,1]

Value : C_NO3 [0,soil_column,Advective Zone,0.01]

Value : C_NO3 [0,soil_column,Advective Zone,0.2]

Value : C_NO3 [0,soil_column,Advective Zone,0.4]

Value : C_NO3 [0,soil_column,Advective Zone,0.6]

Value : C_NO3 [0,soil_column,Advective Zone,0.8]

C_NO3_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_NO3 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_NO3 [0,soil_column,Advective Zone,1]

Value : C_NO3 [0,soil_column,Advective Zone,365]

Value : C_NO3 [0,soil_column,Advective Zone,730]

Value : C_NO3 [0,soil_column,Advective Zone,1095]

Value : C_NO3 [0,soil_column,Advective Zone,1460]

Value : C_NO3 [0,soil_column,Advective Zone,1825]

Value : C_NO3 [0,soil_column,Advective Zone,2190]

Value : C_NO3 [0,soil_column,Advective Zone,2555]

Value : C_NO3 [0,soil_column,Advective Zone,2920]

Value : C_NO3 [0,soil_column,Advective Zone,3285]

Value : C_NO3 [0,soil_column,Advective Zone,3650]

C_O2: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_O2 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_O2 [0,soil_column,Advective Zone,1]

Value : C_O2 [0,soil_column,Advective Zone,0]

Value : C_O2 [0,soil_column,Advective Zone,2]

C_O2_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_O2 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_O2 [0,soil_column,Advective Zone,1]

Value : C_O2 [0,soil_column,Advective Zone,365]

Value : C_O2 [0,soil_column,Advective Zone,730]

Value : C_O2 [0,soil_column,Advective Zone,1095]

Value : C_O2 [0,soil_column,Advective Zone,1460]

Value : C_O2 [0,soil_column,Advective Zone,1825]

Value : C_O2 [0,soil_column,Advective Zone,2190]

Value : C_O2 [0,soil_column,Advective Zone,2555]

Value : C_O2 [0,soil_column,Advective Zone,2920]

Value : C_O2 [0,soil_column,Advective Zone,3285]

Value : C_O2 [0,soil_column,Advective Zone,3650]

C_SO4: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_SO4 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_SO4 [0,soil_column,Advective Zone,1]

Value : C_SO4 [0,soil_column,Advective Zone,0.1]

Value : C_SO4 [0,soil_column,Advective Zone,2]

C_SO4_1: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_SO4 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_SO4 [0,soil_column,Advective Zone,1]

Value : C_SO4 [0,soil_column,Advective Zone,0.01]

Value : C_SO4 [0,soil_column,Advective Zone,0.1]

Value : C_SO4 [0,soil_column,Advective Zone,0.2]

Value : C_SO4 [0,soil_column,Advective Zone,0.5]

Value : C_SO4 [0,soil_column,Advective Zone,1.5]

C_SO4_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_SO4 / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_SO4 [0,soil_column,Advective Zone,1]

Value : C_SO4 [0,soil_column,Advective Zone,365]

Value : C_SO4 [0,soil_column,Advective Zone,730]

Value : C_SO4 [0,soil_column,Advective Zone,1095]

Value : C_SO4 [0,soil_column,Advective Zone,1460]

Value : C_SO4 [0,soil_column,Advective Zone,1825]

Value : C_SO4 [0,soil_column,Advective Zone,2190]

Value : C_SO4 [0,soil_column,Advective Zone,2555]

Value : C_SO4 [0,soil_column,Advective Zone,2920]

Value : C_SO4 [0,soil_column,Advective Zone,3285]

Value : C_SO4 [0,soil_column,Advective Zone,3650]

C_TPH: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: C_TPH / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_TPH [0,soil_column,Advective Zone,1]

Value : C_TPH [0,soil_column,Advective Zone,0.01]

Value : C_TPH [0,soil_column,Advective Zone,2]

Value : C_TPH [0,soil_column,Advective Zone,0.1]

Value : C_TPH [0,soil_column,Advective Zone,0.2]

Value : C_TPH [0,soil_column,Advective Zone,0.4]

Value : C_TPH [0,soil_column,Advective Zone,0.6]

Value : C_TPH [0,soil_column,Advective Zone,0.8]

C_TPH_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: C_TPH / mg/L

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : C_TPH [0,soil_column,Advective Zone,1]

Value : C_TPH [0,soil_column,Advective Zone,365]

Value : C_TPH [0,soil_column,Advective Zone,730]

Value : C_TPH [0,soil_column,Advective Zone,1095]

Value : C_TPH [0,soil_column,Advective Zone,1460]

Value : C_TPH [0,soil_column,Advective Zone,1825]

Value : C_TPH [0,soil_column,Advective Zone,2190]

Value : C_TPH [0,soil_column,Advective Zone,2555]

Value : C_TPH [0,soil_column,Advective Zone,2920]

Value : C_TPH [0,soil_column,Advective Zone,3285]

Value : C_TPH [0,soil_column,Advective Zone,3650]

S_FeIII: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_FeIII / g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_FeIII [0,soil_column,Advective Zone,1]

Value : S_FeIII [0,soil_column,Advective Zone,0.1]

Value : S_FeIII [0,soil_column,Advective Zone,2]

S_FeIII_1: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_FeIII / g/Kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_FeIII [0,soil_column,Advective Zone,1]

Value : S_FeIII [0,soil_column,Advective Zone,0.01]

Value : S_FeIII [0,soil_column,Advective Zone,0.1]

Value : S_FeIII [0,soil_column,Advective Zone,0.2]

Value : S_FeIII [0,soil_column,Advective Zone,0.5]

Value : S_FeIII [0,soil_column,Advective Zone,1.5]

S_FeIII_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: S_FeIII/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_FeIII [0,soil_column,Advective Zone,1]

Value : S_FeIII [0,soil_column,Advective Zone,365]

Value : S_FeIII [0,soil_column,Advective Zone,730]

Value : S_FeIII [0,soil_column,Advective Zone,1095]

Value : S_FeIII [0,soil_column,Advective Zone,1460]

Value : S_FeIII [0,soil_column,Advective Zone,1825]

Value : S_FeIII [0,soil_column,Advective Zone,2190]

Value : S_FeIII [0,soil_column,Advective Zone,2555]

Value : S_FeIII [0,soil_column,Advective Zone,2920]

Value : S_FeIII [0,soil_column,Advective Zone,3285]

Value : S_FeIII [0,soil_column,Advective Zone,3650]

S_NO3: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_NO3 / g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_NO3 [0,soil_column,Advective Zone,1]

Value : S_NO3 [0,soil_column,Advective Zone,0.1]

Value : S_NO3 [0,soil_column,Advective Zone,2]

S_NO3_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: S_NO3/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_NO3 [0,soil_column,Advective Zone,1]

Value : S_NO3 [0,soil_column,Advective Zone,365]

Value : S_NO3 [0,soil_column,Advective Zone,730]

Value : S_NO3 [0,soil_column,Advective Zone,1095]

Value : S_NO3 [0,soil_column,Advective Zone,1460]

Value : S_NO3 [0,soil_column,Advective Zone,1825]

Value : S_NO3 [0,soil_column,Advective Zone,2190]

Value : S_NO3 [0,soil_column,Advective Zone,2555]

Value : S_NO3 [0,soil_column,Advective Zone,2920]

Value : S_NO3 [0,soil_column,Advective Zone,3285]

Value : S_NO3 [0,soil_column,Advective Zone,3650]

S_SO4: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_SO4 / g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_SO4 [0,soil_column,Advective Zone,1]

Value : S_SO4 [0,soil_column,Advective Zone,0.1]

Value : S_SO4 [0,soil_column,Advective Zone,2]

S_SO4_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: S_SO4/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_SO4 [0,soil_column,Advective Zone,1]

Value : S_SO4 [0,soil_column,Advective Zone,365]

Value : S_SO4 [0,soil_column,Advective Zone,730]

Value : S_SO4 [0,soil_column,Advective Zone,1095]

Value : S_SO4 [0,soil_column,Advective Zone,1460]

Value : S_SO4 [0,soil_column,Advective Zone,1825]

Value : S_SO4 [0,soil_column,Advective Zone,2190]

Value : S_SO4 [0,soil_column,Advective Zone,2555]

Value : S_SO4 [0,soil_column,Advective Zone,2920]

Value : S_SO4 [0,soil_column,Advective Zone,3285]

Value : S_SO4 [0,soil_column,Advective Zone,3650]

S_TPH: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_TPH/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_TPH [0,soil_column,Advective Zone,1]

Value : S_TPH [0,soil_column,Advective Zone,0.1]

Value : S_TPH [0,soil_column,Advective Zone,2]

S_TPH_1: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: S_TPH / g/Kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_TPH [0,soil_column,Advective Zone,1]

Value : S_TPH [0,soil_column,Advective Zone,0.01]

Value : S_TPH [0,soil_column,Advective Zone,2]

Value : S_TPH [0,soil_column,Advective Zone,0.1]

Value : S_TPH [0,soil_column,Advective Zone,0.2]

Value : S_TPH [0,soil_column,Advective Zone,0.4]

Value : S_TPH [0,soil_column,Advective Zone,0.6]

Value : S_TPH [0,soil_column,Advective Zone,0.8]

S_TPH_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: S_C16_H34/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : S_TPH [0,soil_column,Advective Zone,1]
 Value : S_TPH [0,soil_column,Advective Zone,365]
 Value : S_TPH [0,soil_column,Advective Zone,730]
 Value : S_TPH [0,soil_column,Advective Zone,1095]
 Value : S_TPH [0,soil_column,Advective Zone,1460]
 Value : S_TPH [0,soil_column,Advective Zone,1825]
 Value : S_TPH [0,soil_column,Advective Zone,2190]
 Value : S_TPH [0,soil_column,Advective Zone,2555]
 Value : S_TPH [0,soil_column,Advective Zone,2920]
 Value : S_TPH [0,soil_column,Advective Zone,3285]
 Value : S_TPH [0,soil_column,Advective Zone,3650]

X_aer: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: X_aer / g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_aer [0,soil_column,Advective Zone,1]

Value : X_aer [0,soil_column,Advective Zone,0.1]

Value : X_aer [0,soil_column,Advective Zone,2]

X_aer_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: X_aer/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_aer [0,soil_column,Advective Zone,1]

Value : X_aer [0,soil_column,Advective Zone,365]

Value : X_aer [0,soil_column,Advective Zone,730]

Value : X_aer [0,soil_column,Advective Zone,1095]

Value : X_aer [0,soil_column,Advective Zone,1460]

Value : X_aer [0,soil_column,Advective Zone,1825]

Value : X_aer [0,soil_column,Advective Zone,2190]

Value : X_aer [0,soil_column,Advective Zone,2555]

Value : X_aer [0,soil_column,Advective Zone,2920]

Value : X_aer [0,soil_column,Advective Zone,3285]

Value : X_aer [0,soil_column,Advective Zone,3650]

X_den: Description:

Abscissa: Time

Title:

Abscissa Label: time / d

Ordinate Label: X_anaer / g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_den [0,soil_column,Advective Zone,1]

Value : X_den [0,soil_column,Advective Zone,0.1]

Value : X_den [0,soil_column,Advective Zone,2]

X_den_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: X_anae/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_den [0,soil_column,Advective Zone,1]

Value : X_den [0,soil_column,Advective Zone,365]

Value : X_den [0,soil_column,Advective Zone,730]

Value : X_den [0,soil_column,Advective Zone,1095]

Value : X_den [0,soil_column,Advective Zone,1460]

Value : X_den [0,soil_column,Advective Zone,1825]

Value : X_den [0,soil_column,Advective Zone,2190]

Value : X_den [0,soil_column,Advective Zone,2555]

Value : X_den [0,soil_column,Advective Zone,2920]

Value : X_den [0,soil_column,Advective Zone,3285]

Value : X_den [0,soil_column,Advective Zone,3650]

X_irb_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: X_anae/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_irb [0,soil_column,Advective Zone,1]

Value : X_irb [0,soil_column,Advective Zone,365]

Value : X_irb [0,soil_column,Advective Zone,730]

Value : X_irb [0,soil_column,Advective Zone,1095]

Value : X_irb [0,soil_column,Advective Zone,1460]

Value : X_irb [0,soil_column,Advective Zone,1825]

Value : X_irb [0,soil_column,Advective Zone,2190]

Value : X_irb [0,soil_column,Advective Zone,2555]

Value : X_irb [0,soil_column,Advective Zone,2920]

Value : X_irb [0,soil_column,Advective Zone,3285]

Value : X_irb [0,soil_column,Advective Zone,3650]

X_met_depth: Description:

Abscissa: Space

Title:

Abscissa Label: depth / m

Ordinate Label: X_anae/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_met [0,soil_column,Advective Zone,1]

Value : X_met [0,soil_column,Advective Zone,365]

Value : X_met [0,soil_column,Advective Zone,730]

Value : X_met [0,soil_column,Advective Zone,1095]

Value : X_met [0,soil_column,Advective Zone,1460]

Value : X_met [0,soil_column,Advective Zone,1825]

Value : X_met [0,soil_column,Advective Zone,2190]

Value : X_met [0,soil_column,Advective Zone,2555]

Value : X_met [0,soil_column,Advective Zone,2920]

Value : X_met [0,soil_column,Advective Zone,3285]

Value : X_met [0,soil_column,Advective Zone,3650]

X_srb_depth: Description:

Abcissa: Space

Title:

Abcissa Label: depth / m

Ordinate Label: X_anae/ g/kg

Curves:

Type : Variable [CalcNum,Comp.,Zone,Time/Space]

Value : X_srb [0,soil_column,Advective Zone,1]

Value : X_srb [0,soil_column,Advective Zone,365]

Value : X_srb [0,soil_column,Advective Zone,730]

Value : X_srb [0,soil_column,Advective Zone,1095]

Value : X_srb [0,soil_column,Advective Zone,1460]

Value : X_srb [0,soil_column,Advective Zone,1825]

Value : X_srb [0,soil_column,Advective Zone,2190]

Value : X_srb [0,soil_column,Advective Zone,2555]

Value : X_srb [0,soil_column,Advective Zone,2920]

Value : X_srb [0,soil_column,Advective Zone,3285]

Value : X_srb [0,soil_column,Advective Zone,3650]

Calculation Parameters

Numerical Parameters: Maximum Int. Step Size: 8

Maximum Integrat. Order: 5

Number of Codiagonals: 100

Maximum Number of Steps: 1000

Fit Method: secant

Max. Number of Iterat.: 100
