Chesapeake Bay Sediment Flux Model

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Chesapeake Bay Program
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IAN Annapolis Office, Large Conference Room.
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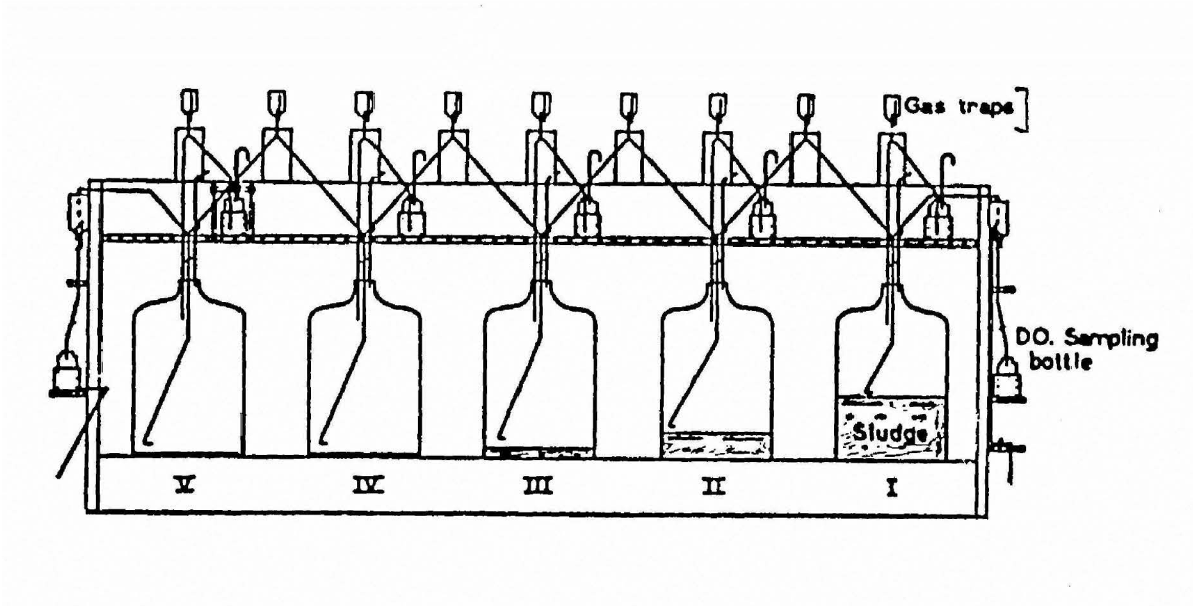
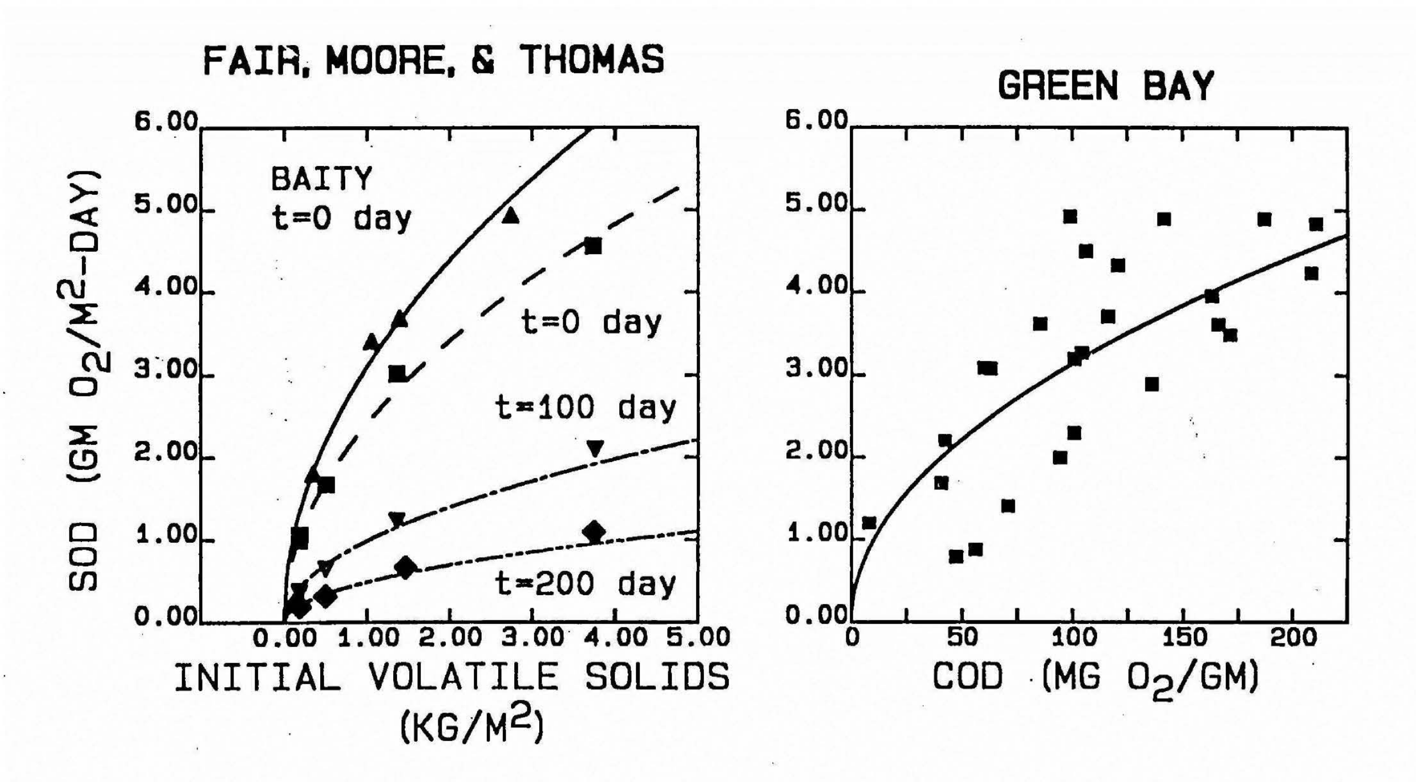
Sediment Oxygen Demand

Fair, Moore, and Thomas 1941





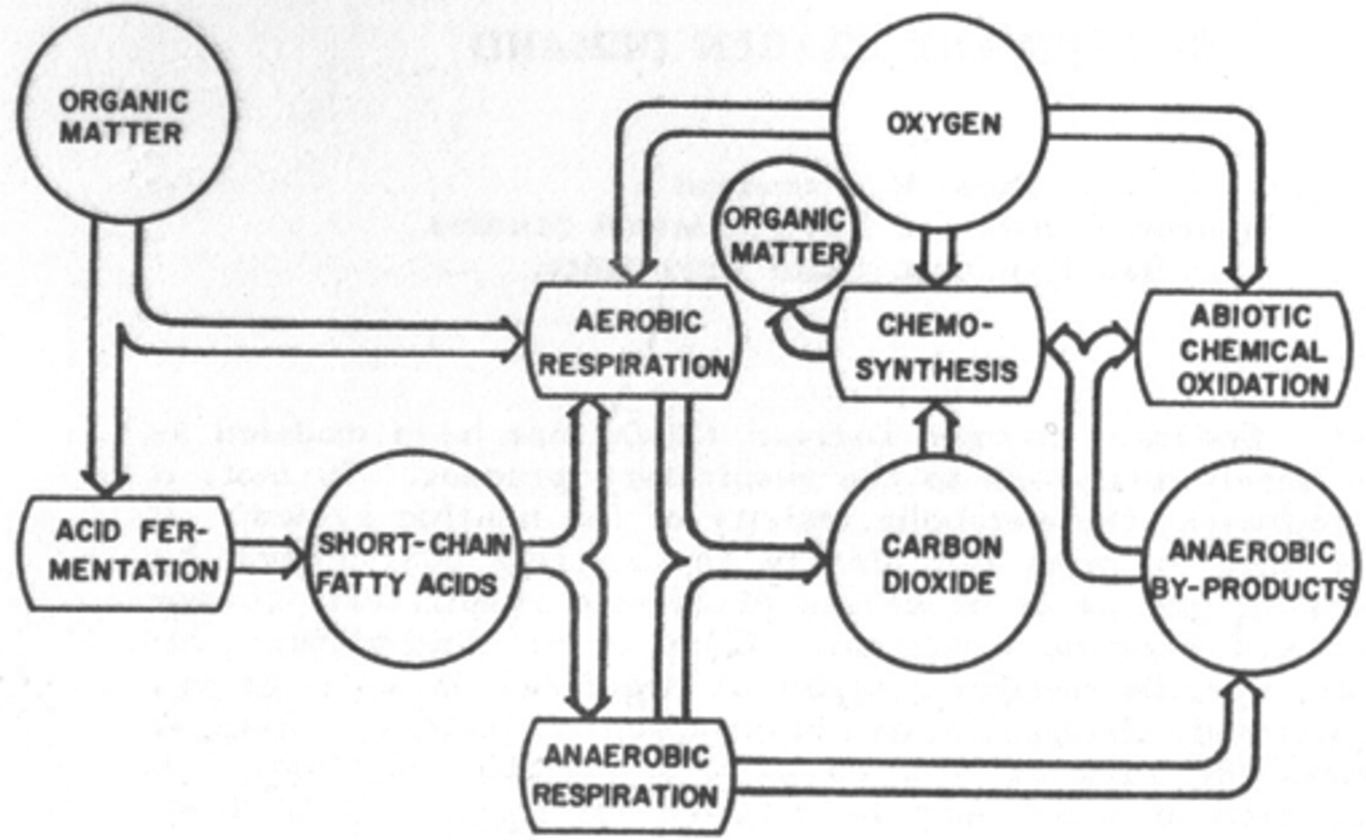


Figure 1. The relationship among oxygen-consuming and anaerobic benthic processes. Aerobic respiration and chemosynthesis are both oxygen-consuming processes, but the latter is accompanied by carbon dioxide uptake while respiration produces carbon dioxide. Oxidation of sulfides, ferrous, manganous, etc., by chemosynthetic organisms has not been distinguished from abiotic chemical oxidation.

Pamatmat (1986). Problems with empirical models of sediment oxygen demand. Sediment Oxygen Demand. Processes, Modeling and Measurement. K. J. Hatcher., Institute of Natural Resources, University of Georgia, Athens, GA.: 23-37.

TABLE 1. Oxygen-Consuming Processes in Sediment and Environmental Variables that Affect Sediment Oxygen Uptake

Oxygen-Consuming Processes	Environmental Variables
Biological Oxidation	Oxygen Pressure
Aerobic Respiration	Temperature
$(CH_2O)_n \rightarrow CO_2$	Salinity
Sulfide Oxidation	Light
$S^{2-} \rightarrow S^o \rightarrow S_2O_3^{2-} \rightarrow SO_4^{2-}$	
	Hydrostatic Pressure
Nitrification	
$NH_3 \rightarrow NO_2^- \rightarrow NO_3^-$	Turbulence
Iron Oxidation	Sediment Properties
	Grain size
$Fe^{2+} \rightarrow Fe^{3+}$	Organic matter content
Methane Oxidation	
$CH_4 \rightarrow CH_3OH \rightarrow CO_2$	Rate of Organic Matter Supply
	Primary productivity
Abiotic Chemical Oxidation	Sedimentation rate
	Organic pollution
$S^{2-} \rightarrow SO_4^{2-}$	
$Fe^{2-} \rightarrow Fe^{3+}$	Chemical Pollution
	Industrial
$Mn^{2+} \rightarrow Mn^{4+}$	Agricultural
	Domestic
Others	Community Structure

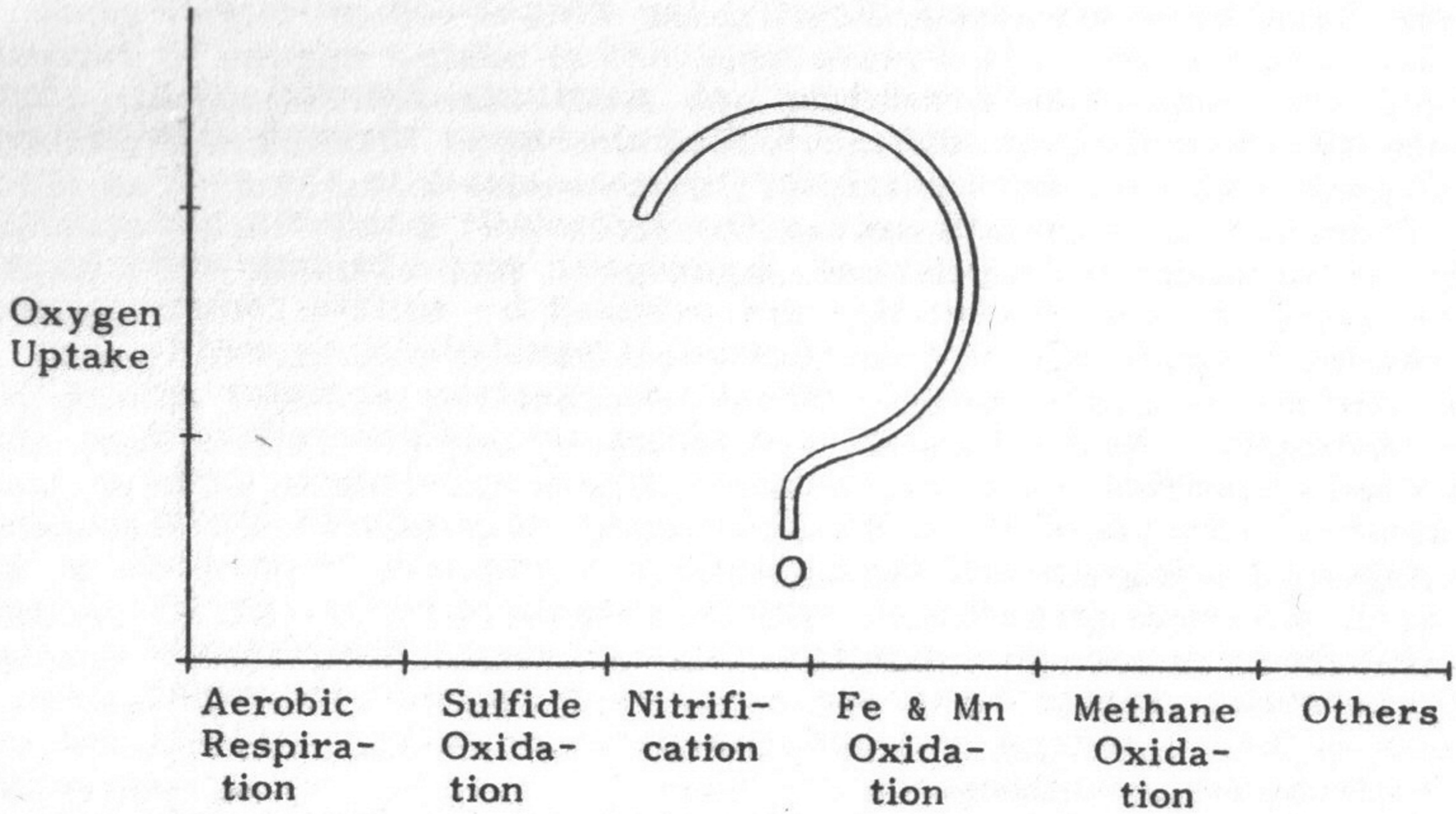


Figure 2. Curve summarizing present knowledge of SOD as an integral of the different oxygen consuming processes.

Pamatmat (1986). Problems with empirical models of sediment oxygen demand. Sediment Oxygen Demand. Processes, Modeling and Measurement. K. J. Hatcher., Institute of Natural Resources, University of Georgia, Athens, GA.: 23-37.

Sediment Flux Model
Sediment Diagenesis = Sediment Flux

- Flux of organic matter to the sediment is the source

- Fluxes are proportional to the stoichiometry of the decaying organic matter (Redfield stoichiometry)

$$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4)$$

Ratio of fluxes

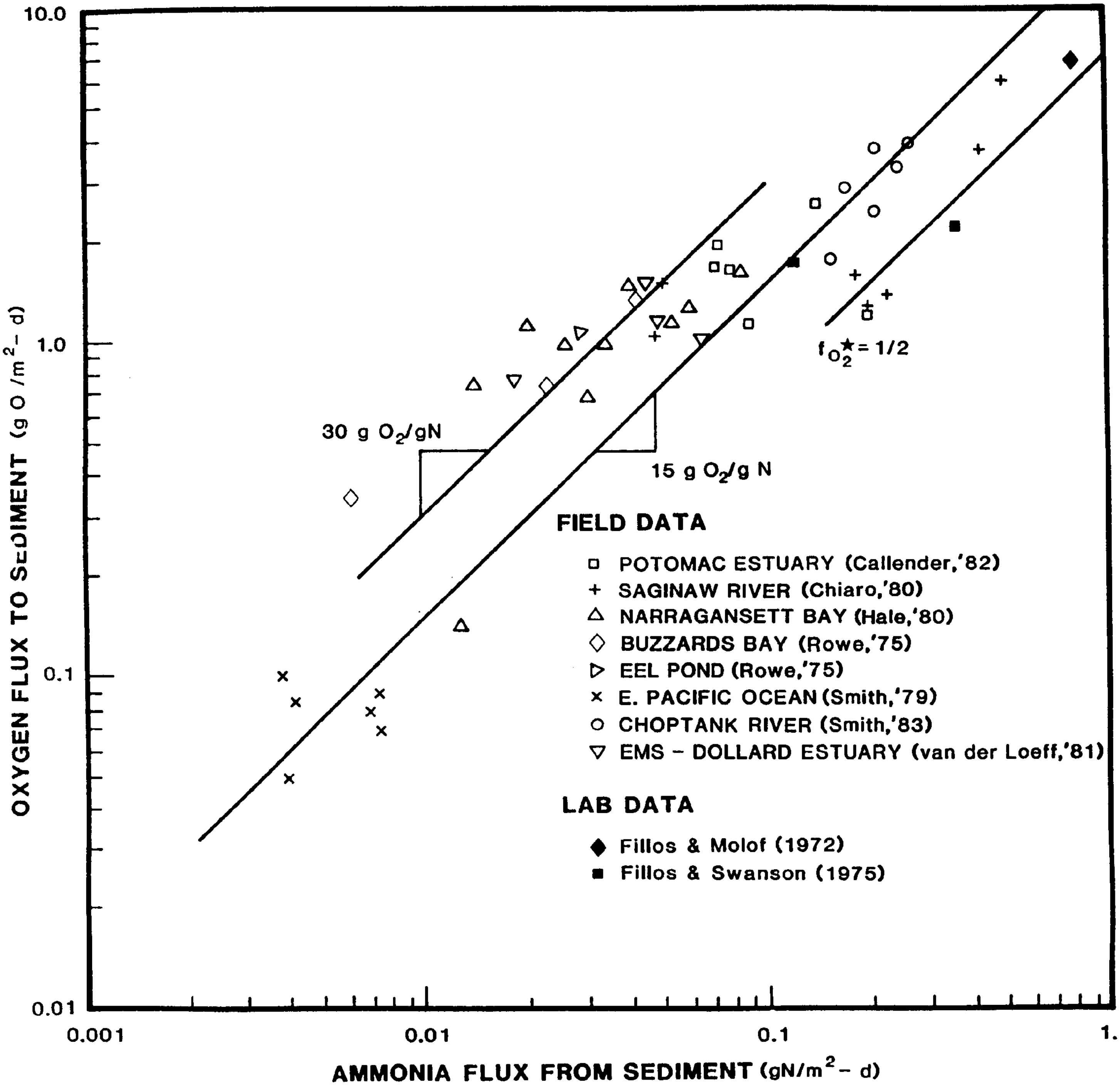
$$\frac{\text{SOD}}{\text{NH}_3} = \frac{106\ (\text{O}_2)}{16\ (\text{N})}\frac{32\ (\text{gO}_2/\text{mol})}{14\ (\text{gN}/\text{mol})} = 15.1\ \text{gO}_2/\text{g N}$$

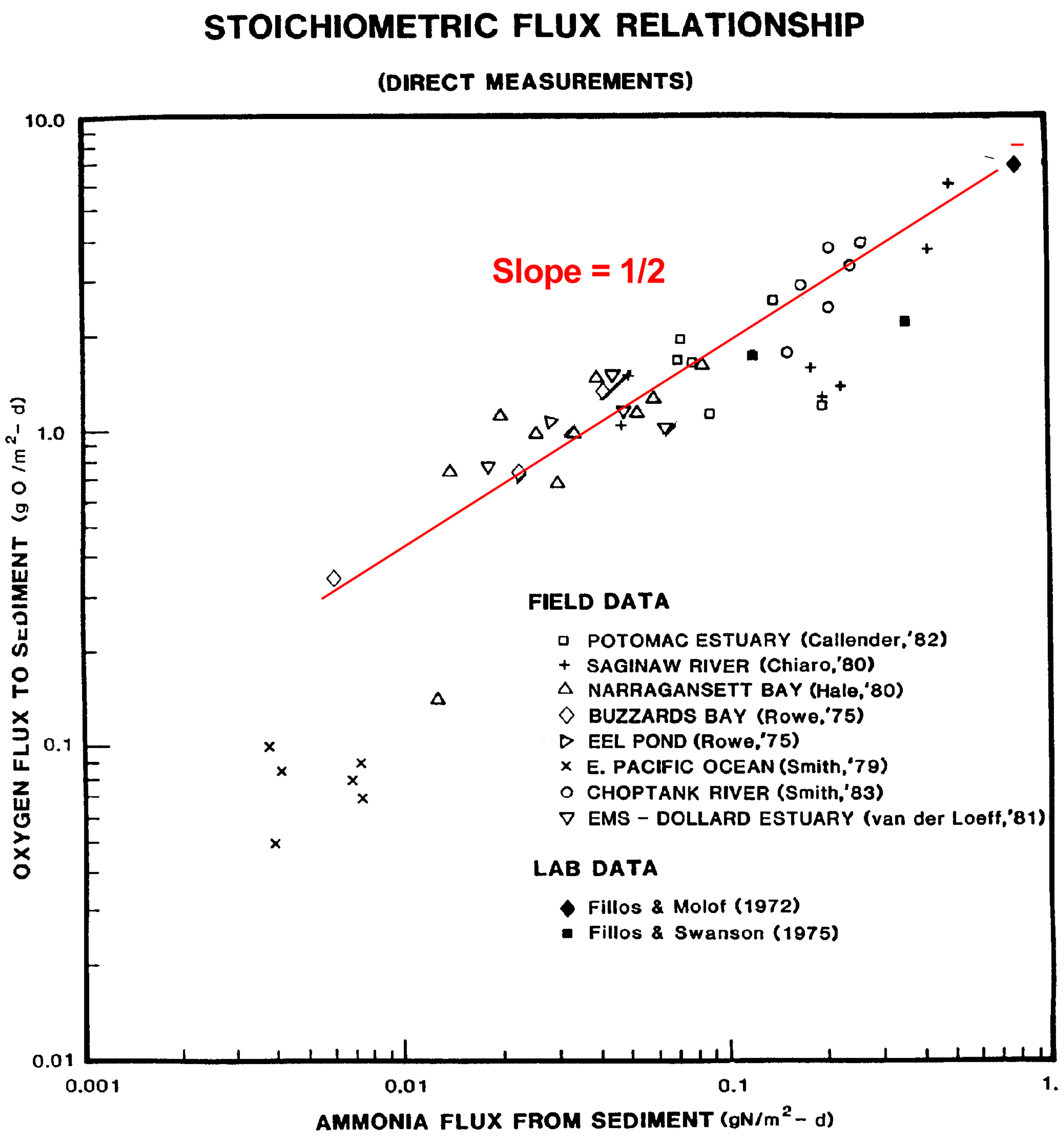
Organic carbon oxidized by O_2

Ammonia conservative

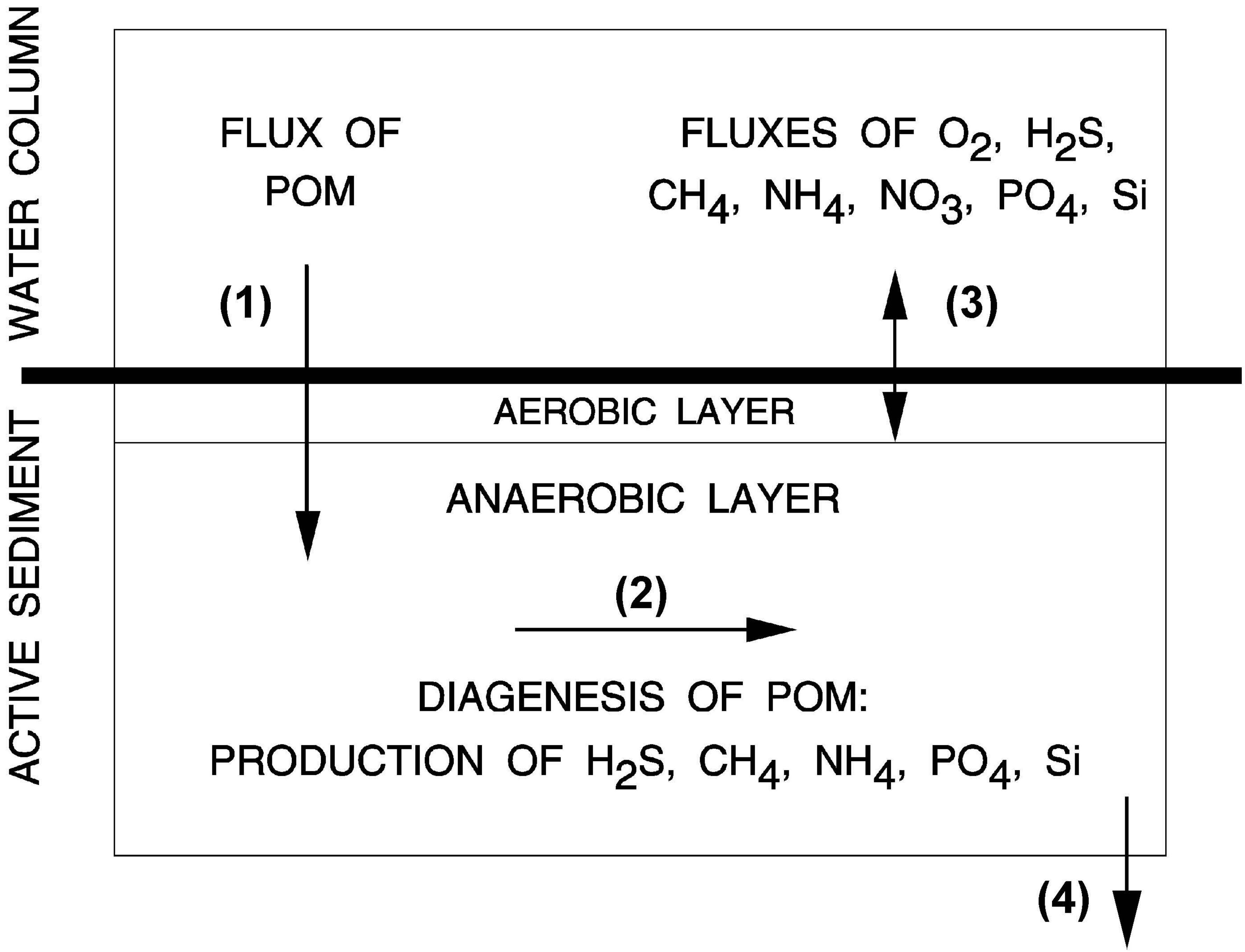
STOICHIOMETRIC FLUX RELATIONSHIP

(DIRECT MEASUREMENTS)



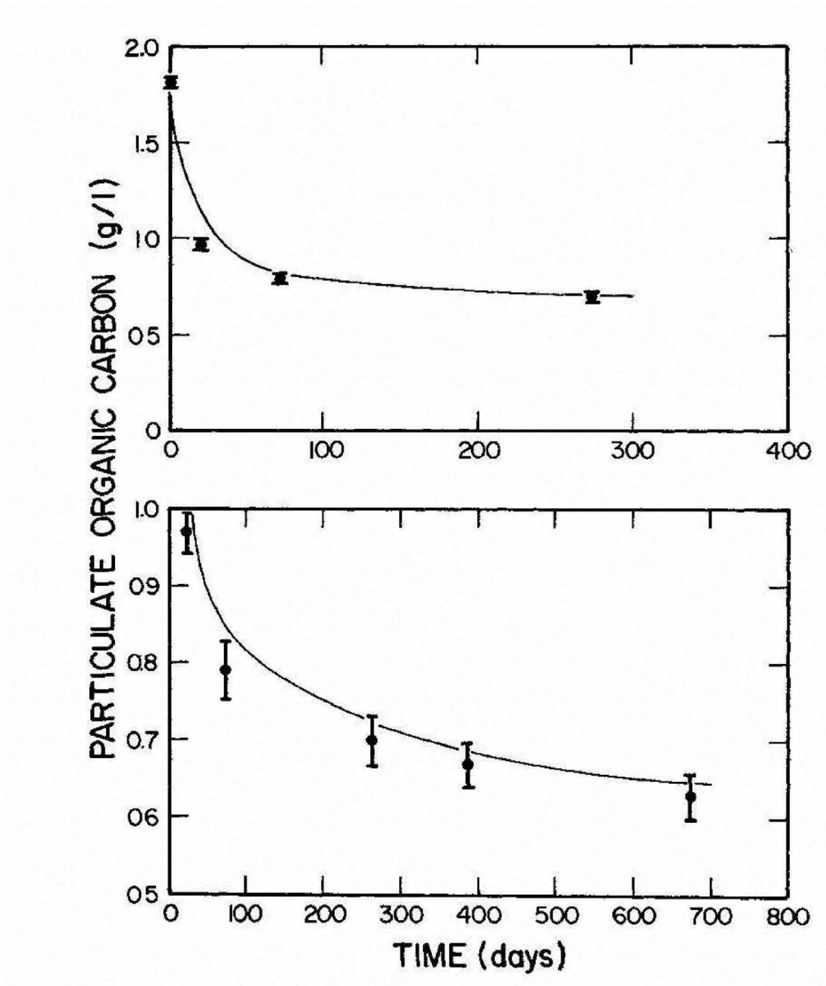

STOICHIOMETRIC FLUX RELATIONSHIP
(DIRECT MEASUREMENTS)
Slope = 1/2
FIELD DATA
POTOMAC ESTUARY (Callender,'82)
SAGINAW RIVER (Chiaro,'80)
NARRAGANSETT BAY (Hale,'80)
BUZZARDS BAY (Rowe,'75)
EEL POND (Rowe,'75)
E. PACIFIC OCEAN (Smith,'79)
CHOPTANK RIVER (Smith,'83)
EMS – DOLLARD ESTUARY (van der Loeff,'81)
LAB DATA
Fillos & Molof (1972)
Fillos & Swanson (1975)
OXYGEN FLUX TO SEDIMENT (g O /m2 – d)
10.0
1.0
0.1
0.01
0.001
0.01
0.1
1.
AMMONIA FLUX FROM SEDIMENT (gN/m2 – d)

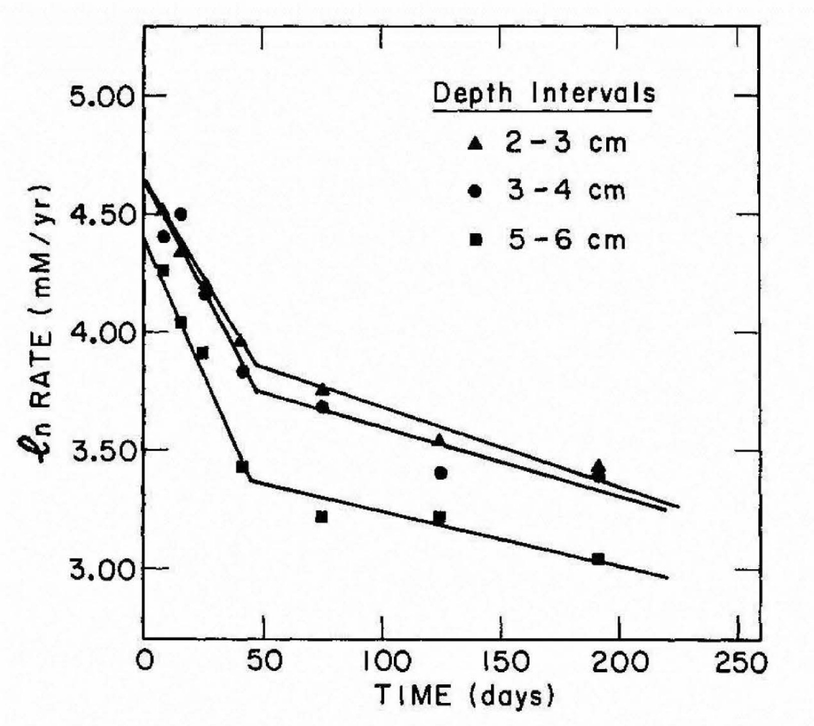
Schematic of Sediment Flux Model

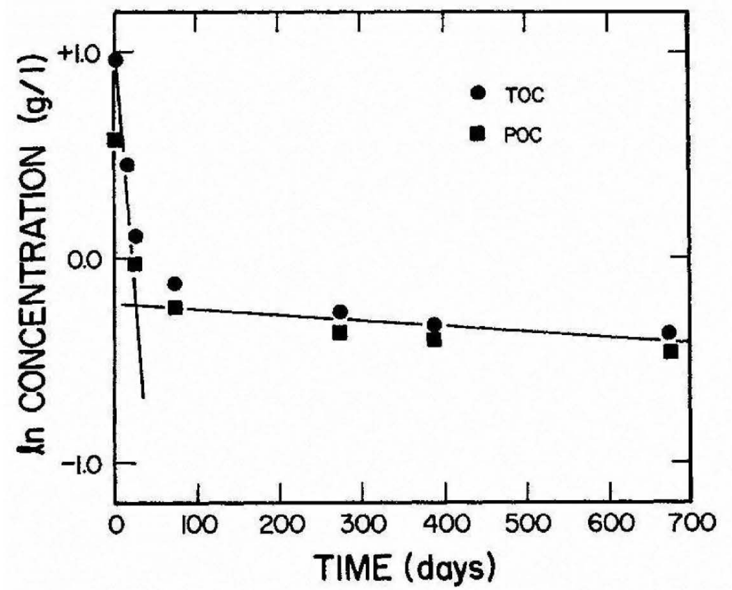


Decay of Organic Matter

$$G_T(t) = G_{01}[\exp(-k_1 t)] + G_{02}[\exp(-k_2 t)] + G_{NR}$$







The Role of Sedimentary Organic Matter
in Bacterial Sulfate Reduction:
The G Model Tested
Westrich and Berner
Limnology and Oceanography, Vol. 29, No. 2 , pp. 236-249

Sediment Diagenesis Model - Three G Model

- Diagenesis is the decay or decomposition of POM in the sediment bed
- The SFM uses Berner's 3G model framework, essentially splitting the deposited POM into labile (G_1), refractory (G_2), and inert (G3) pools

POC	G_1	G_2	G_3
f_{POC}	0.65	0.20	0.15
k_{diag} (/day)	0.035	0.0018	0.0
1 "e-folding" (days)	28	555	
2 (Temp correction)	1.10	1.15	

θ	Q10 = k(10)/k(20)
1.068	0.518
1.100	0.386
1.150	0.247
k10 = k20	θ^(-10)

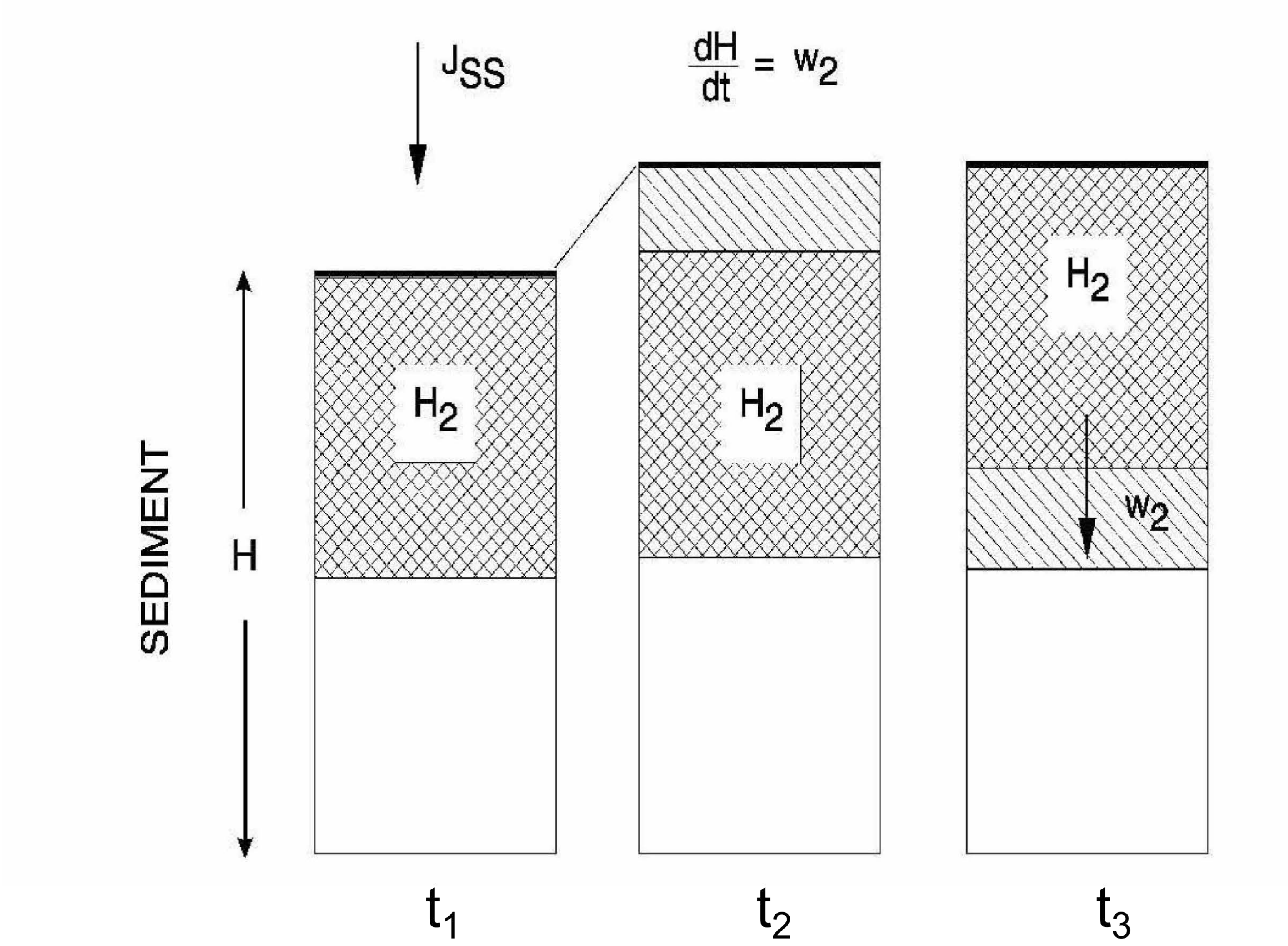
POC Mass Balance Equation

$$H\,\frac{dPOC_i}{dt} = f_{POC_i} J_{POC} - w_2 POC_i - H \cdot k_{POC_i} \theta_{POC_i} POC_i$$

where

- H = depth of sediment (10 cm)
- POC_i = concentration of POC in pool G_i
- f_{POCi} = fraction of deposited POC going to G_i
- J_{POC} = deposition rate of POC (g C/m^2-day)
- w_2 = burial rate of organic matter (m/day)
- k_{POCi} = diagenesis or decay rate of POC_i
- 2_{POCi} = temperature correction factor

Model of Sediment Loss by Burial



Steady State Solution for POC Concentrations

$$H\frac{dPOC_i}{dt} = f_{POC_i} J_{POC} - w_2 POC_i - H \cdot k_{POC_i} \theta_{POC_i} POC_i$$

- Rate of diagenesis

$$J_C = \sum_{i=1}^{2} H \cdot k_{POC_i} \theta_{POC_i} POC_i$$

Solutions

G_1 and G_2 $$POC_i = \frac{f_{POC_i} J_{POC}}{k_i H + w_2}$$

G_3 $$POC_i = \frac{f_{POC_i} J_{POC}}{w_2}$$

Magnitudes of the Parameters
Resulting Concentrations

G_1 and G_2 $$POC_i = \frac{f_{POC_i} J_{POC}}{k_i H + w_2}$$ G_3 $$POC_i = \frac{f_{POC_i} J_{POC}}{w_2}$$

What is the range in w_2?

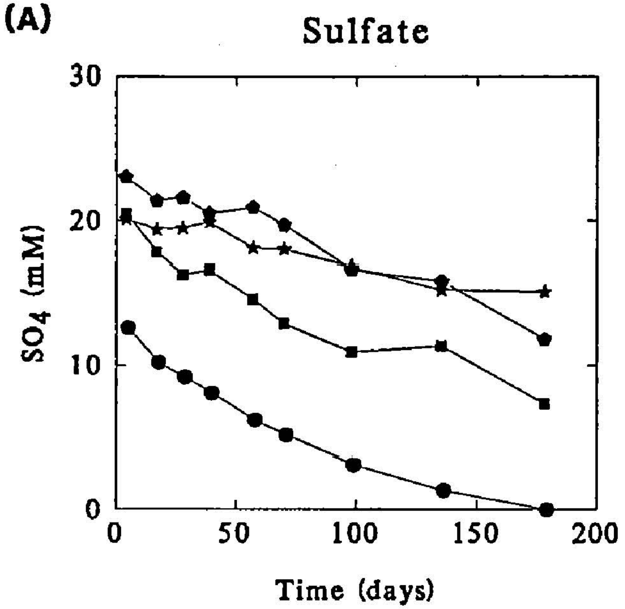
	ocean	bays-estuaries	"high deposition"
w_2 (cm/yr)	0.001-0.01	0.01-1	1-10
	G_1	G_2	
k_iH (cm/yr)	130	6.6	Burial << Diagenesis

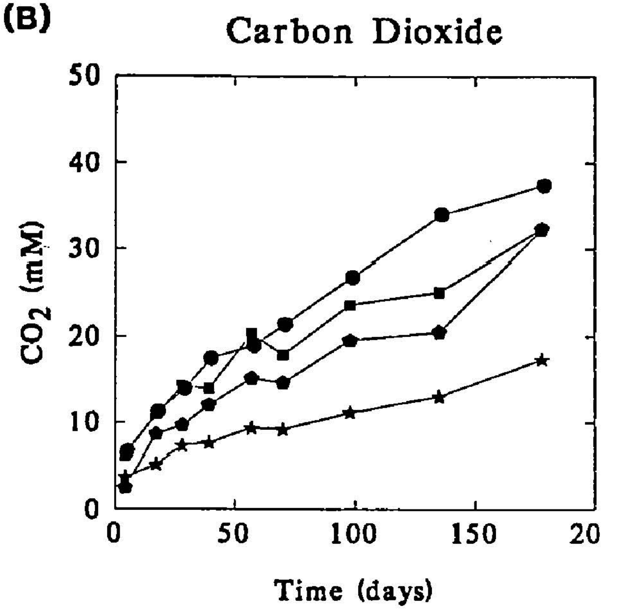
From these coefficients $POC_i = f_{POCi}\ J_{POC} / k_iH$

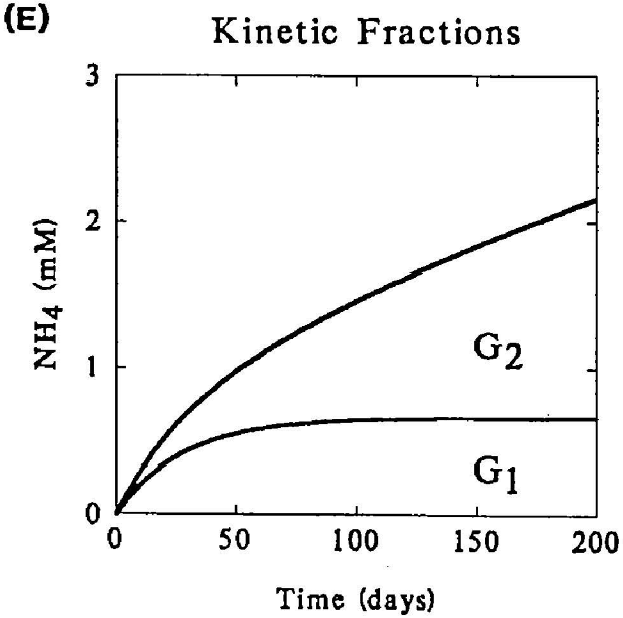
Time to equilibrium: POC_1. 3-4 months POC_2. 5-6 years

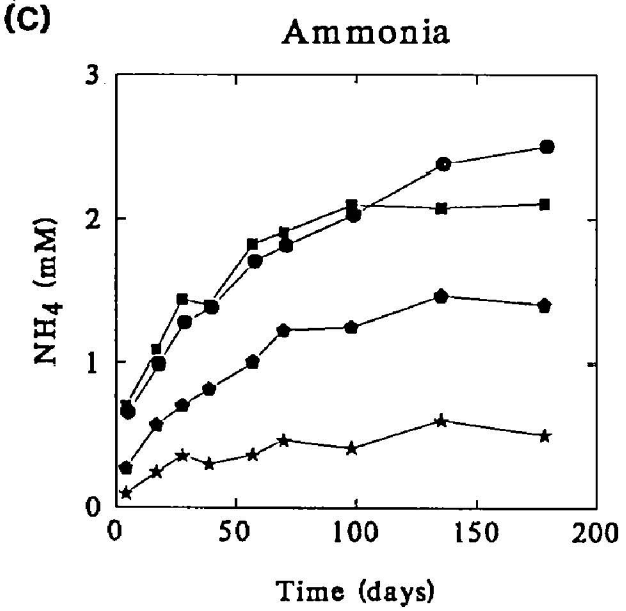
POC_3 = 40 years for w_2 = 0.25 cm/yr

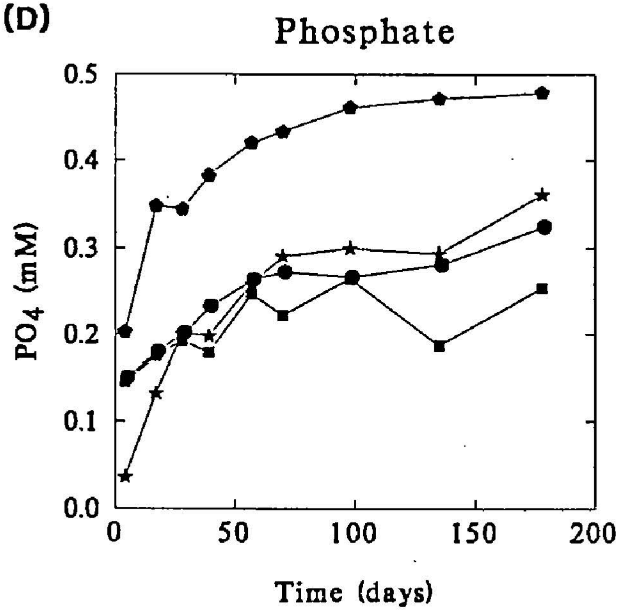
Sediment Mineralization Experiments











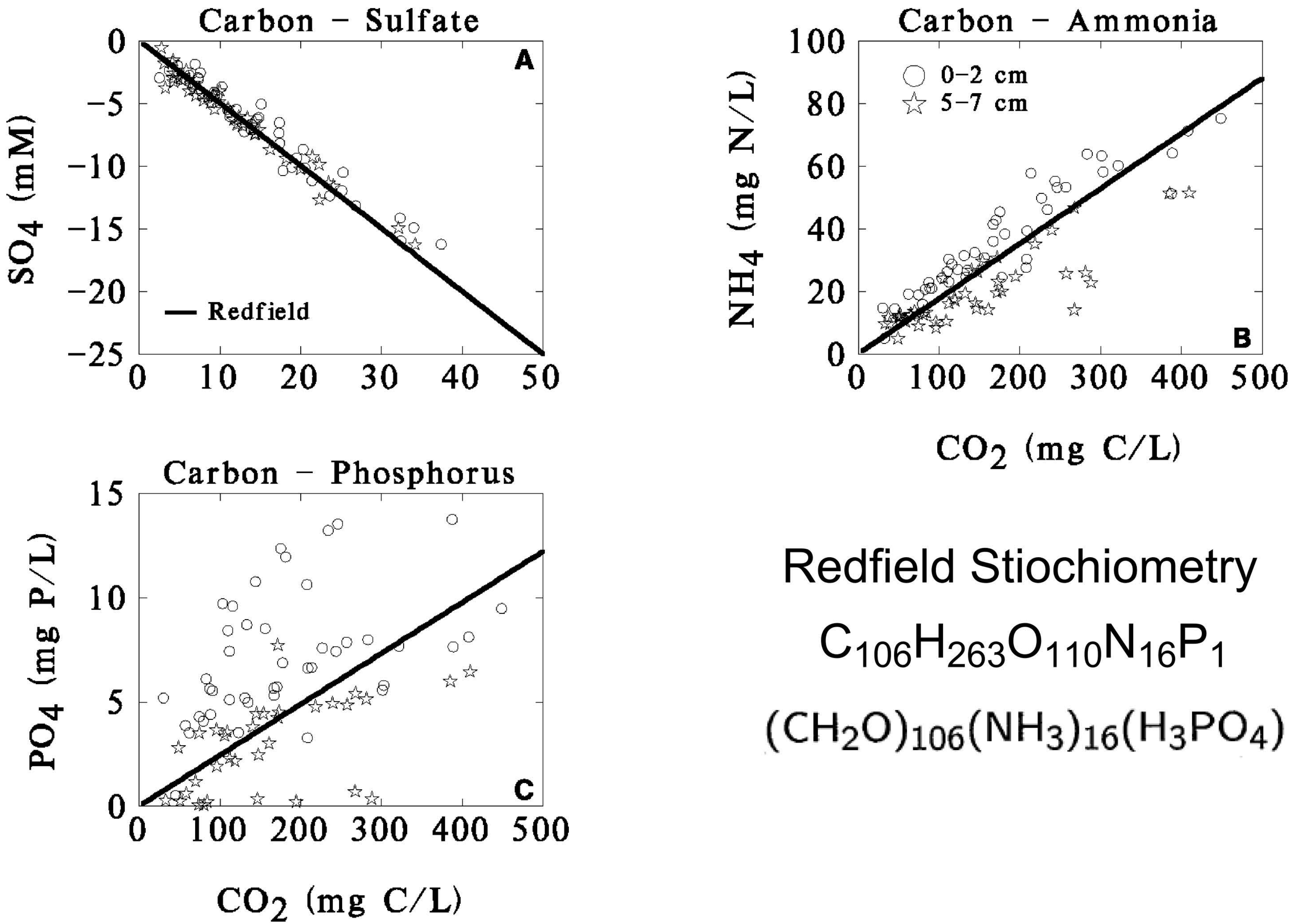
Sediment/Water = 1:3

Legend

- ● Station 17
- ■ Station 21
- ★ Station 25
- ⬟ Station 26

Data from Burdige, 1991

Diagenesis Stoichiometry

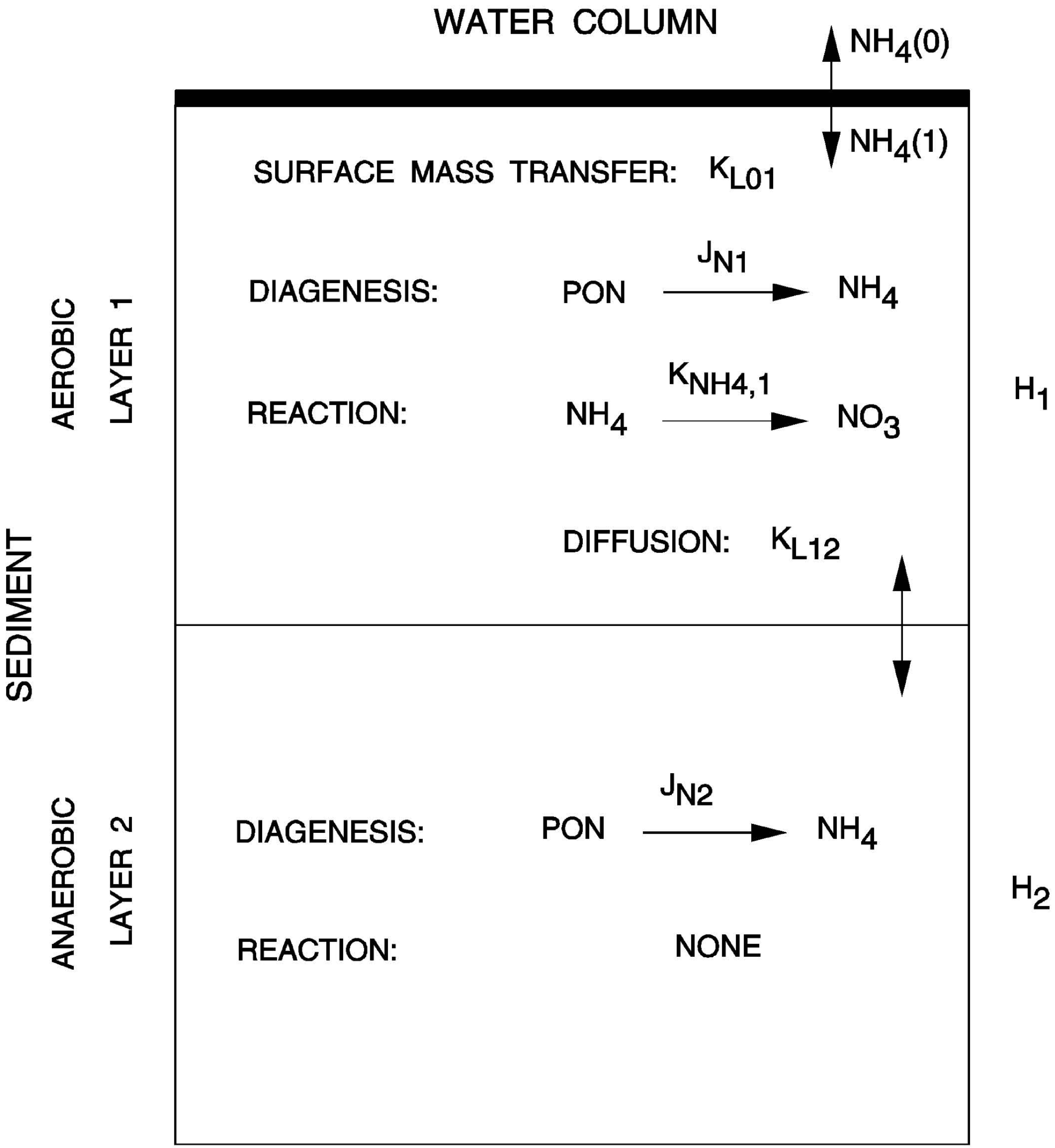


Redfield Stiochiometry

$C_{106}H_{263}O_{110}N_{16}P_1$

$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4)$

Ammonia Flux Model



Aerobic Layer

$$H_1 \frac{d[\mathsf{NH_4(1)}]}{dt} = -k_{\mathsf{NH_4,1}}[\mathsf{NH_4(1)}]H_1$$
$$-K_{\mathsf{L01}}\Big([\mathsf{NH_4(1)}] - [\mathsf{NH_4(0)}]\Big)$$
$$+K_{\mathsf{L12}}\Big([\mathsf{NH_4(2)}] - [\mathsf{NH_4(1)}]\Big) + J_{\mathsf{N1}}$$

Anaerobic Layer

$$H_2 \frac{d[\mathsf{NH_4(2)}]}{dt} =$$
$$-K_{\mathsf{L12}}\Big([\mathsf{NH_4(2)}] - [\mathsf{NH_4(1)}]\Big) + J_{\mathsf{N2}}$$

- H_1 and H_2 = depths of the aerobic (1) and anaerobic (2) layers

- $[NH_4(0)]$, $[NH_4(1)]$, and $[NH_4(2)]$ = ammonia concentrations in overlying water (0),layers (1) and (2)

- $k_{NH_4,1}$ = nitrification rate constant in aerobic layer

Solution

$$
\begin{aligned}
0 &= -k_{\mathrm{NH_4},1}[\mathrm{NH_4(1)}]H_1 \\
&\quad -K_{\mathrm{L01}}\Big([\mathrm{NH_4(1)}]-[\mathrm{NH_4(0)}]\Big)+J_{\mathrm{N1}}+J_{\mathrm{N2}}
\end{aligned}
$$

Ammonia concentrations

$$
[\mathrm{NH_4(1)}]=\frac{J_{\mathrm{N}}+K_{\mathrm{L01}}[\mathrm{NH_4(0)}]}{K_{\mathrm{L01}}+k_{\mathrm{NH_4},1}H_1}
$$

$$
[\mathrm{NH_4(2)}]=\frac{J_{\mathrm{N}}}{K_{\mathrm{L12}}}+[\mathrm{NH_4(1)}]
$$

where $J_{\mathrm{N}}=J_{\mathrm{N1}}+J_{\mathrm{N2}}$

Ammonia flux

$$
J[\mathrm{NH_4}]=K_{\mathrm{L01}}\Big([\mathrm{NH_4(1)}]-[\mathrm{NH_4(0)}]\Big)
$$

or

$$
\begin{aligned}
J[\mathrm{NH_4}] &= J_{\mathrm{N}}\frac{K_{\mathrm{L01}}}{K_{\mathrm{L01}}+k_{\mathrm{NH_4},1}H_1} \\
&\quad -[\mathrm{NH_4(0)}]\left(\frac{1}{K_{\mathrm{L01}}}+\frac{1}{k_{\mathrm{NH_4},1}H_1}\right)^{-1}
\end{aligned}
$$

- K_{L01} = mass transfer coefficient between overlying water and aerobic layer

- K_{L12} = mass transfer coefficient between H_1 and H_2

- J_{N1} and J_{N2} = sources of ammonia layers 1,2 from diagenesis of PON

Surface Mass Transfer Coefficient K_{L01}

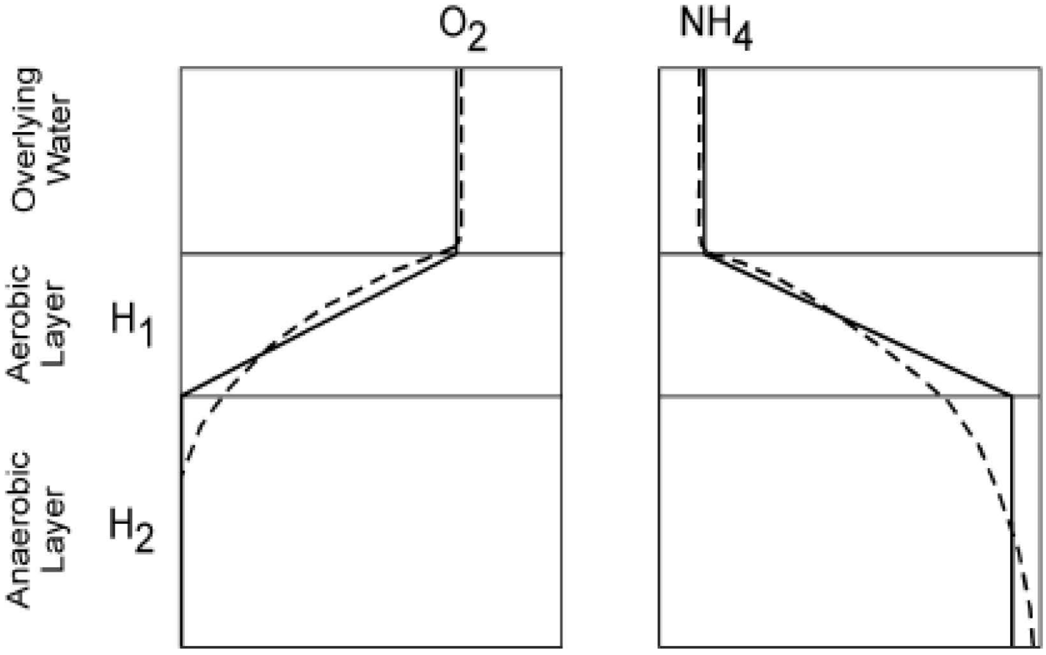


Figure 2: Schematic diagram of the idealized vertical pro files of oxygen and ammonia.

$$
\begin{aligned}
J[\mathrm{NH_4}] &= -D_{\mathrm{NH_4}} \left.\frac{d[\mathrm{NH_4}(z)]}{dz}\right|_{z=0} \\
&\simeq -D_{\mathrm{NH_4}} \frac{[\mathrm{NH_4}(0)] - [\mathrm{NH_4}(H_1)]}{H_1} = \\
&\quad -K_{\mathrm{L01,NH_4}}\Big([\mathrm{NH_4}(0)] - [\mathrm{NH_4}(H_1)]\Big)
\end{aligned}
$$

where

$$K_{\mathrm{L01,NH_4}} = \frac{D_{\mathrm{NH_4}}}{H_1}$$

surface mass transfer coefficient, $D_{\mathrm{NH_4}}$ = diffusion coef- ficient

Surface Mass Transfer Coefficient K_{L01}

Similar argument for the SOD

$$\begin{aligned}\mathsf{SOD} &= D_{\mathsf{O_2}} \left.\frac{d[\mathsf{O_2}(z)]}{dz}\right|_{z=0} \\ &\simeq D_{\mathsf{O_2}} \frac{[\mathsf{O_2}(0)] - [\mathsf{O_2}(H_1)]}{H_1} \\ &= \frac{D_{\mathsf{O_2}}}{H_1}[\mathsf{O_2}(0)] \\ &= K_{\mathsf{L01,O_2}}\Big([\mathsf{O_2}(0)]\Big)\end{aligned}$$

where

$$K_{\mathsf{L01,O_2}} = \frac{D_{\mathsf{O_2}}}{H_1}$$

Therefore

$$K_{\mathsf{L01,O_2}} = \frac{\mathsf{SOD}}{[\mathsf{O_2}(0)]} \triangleq s$$

a measured quantity

Depth of the Aerobic Zone, and Reaction Velocities

Need $k_{\mathsf{NH_4},1}H_1$

$$H_1 = D_{\mathsf{O_2}}\frac{[\mathsf{O_2(0)}]}{\mathsf{SOD}} = \frac{D_{\mathsf{O_2}}}{s}$$

Reaction rate-depth product $k_{\mathsf{NH_4},1}H_1$s

$$k_{\mathsf{NH_4},1}H_1 = \frac{D_{\mathsf{O_2}}k_{\mathsf{NH_4},1}}{s}$$

Define *reaction velocity*

$$\kappa_{\mathsf{NH_4},1} = \sqrt{D_{\mathsf{O_2}}k_{\mathsf{NH_4},1}}$$

Ammonia flux

$$J[\mathsf{NH_4}] = J_{\mathsf{N}}\frac{s^2}{s^2+\kappa^2_{\mathsf{NH_4},1}} - [\mathsf{NH_4(0)}]\left(\frac{1}{s}+\frac{s}{\kappa^2_{\mathsf{NH_4},1}}\right)^{-1}$$

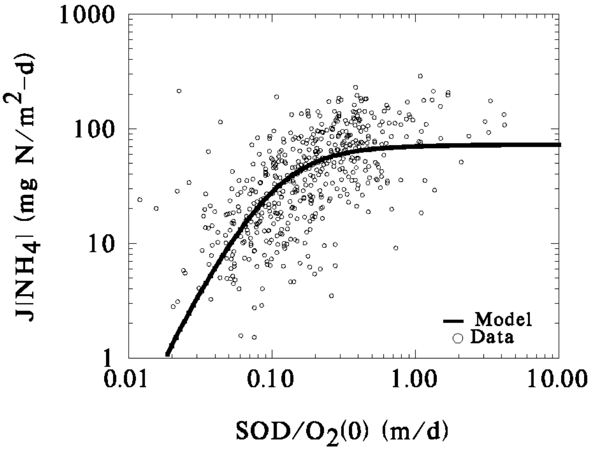


Fig. 3.5 Ammonia flux versus $s = \mathrm{SOD}/[O_2(0)]$ for all stations and times in the Chesapeake Bay data set.

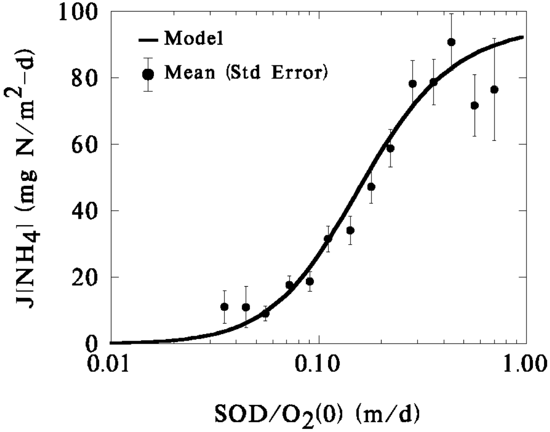


Fig. 3.6 Comparison of model calculation to data grouped into 0.1 $\log_{10}$ intervals of s.

Nitrate Flux Model

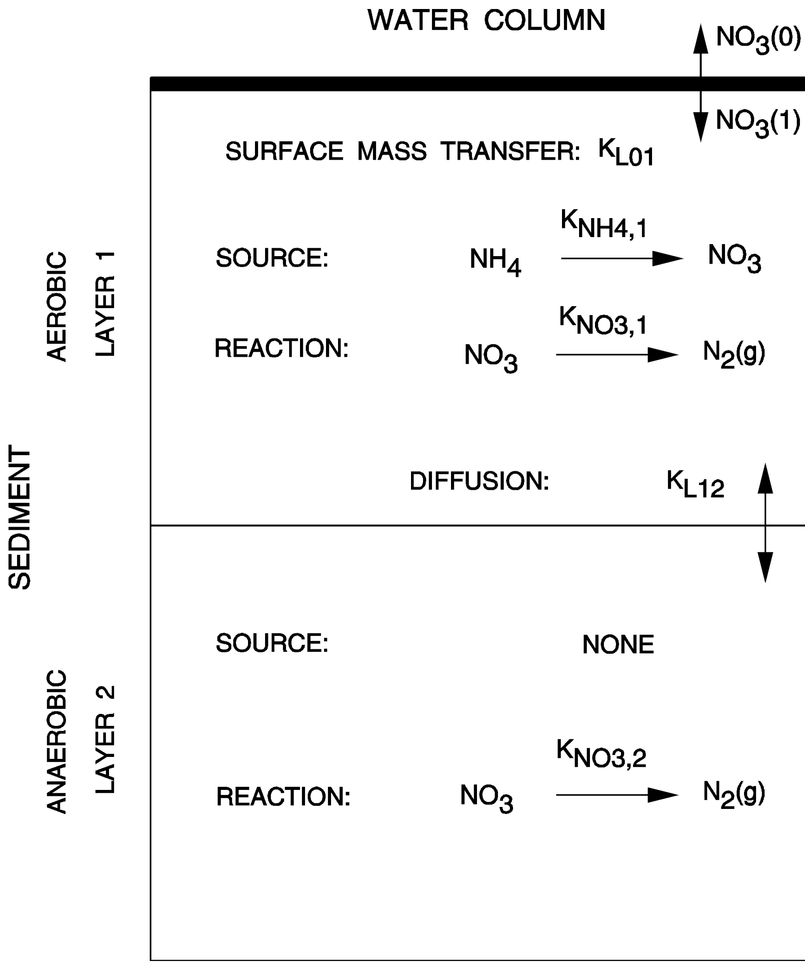


Figure 1: Schematic model of nitrate model

Aerobic Layer

$$
\begin{aligned}
H_1 \frac{d[\mathsf{NO_3(1)}]}{dt} &= -k_{\mathsf{NO_3,1}}[\mathsf{NO_3(1)}]H_1 \\
&\quad -K_{\mathsf{L01}}([\mathsf{NO_3(1)}] - [\mathsf{NO_3(0)}]) \\
&\quad +K_{\mathsf{L12}}([\mathsf{NO_3(2)}] - [\mathsf{NO_3(1)}]) \\
&\quad +S[\mathsf{NO_3}]
\end{aligned}
$$

Anaerobic Layer

$$
\begin{aligned}
H_2 \frac{d[\mathsf{NO_3(2)}]}{dt} &= -k_{\mathsf{NO_3,2}}[\mathsf{NO_3(2)}]H_2 \\
&\quad -K_{\mathsf{L12}}([\mathsf{NO_3(2)}] - [\mathsf{NO_3(1)}])
\end{aligned}
$$

where $S[\mathsf{NO_3}]$ = nitrate from ammonia nitrification

Solutions $[\mathrm{NO_3(1)}] =$

$$\frac{S[\mathrm{NO_3}] + K_{\mathrm{L01}}[\mathrm{NO_3(0)}]}{k_{\mathrm{NO_3,1}}H_1 + K_{\mathrm{L01}} + \left(\frac{1}{k_{\mathrm{NO_3,2}}H_2} + \frac{1}{K_{\mathrm{L12}}}\right)^{-1}}$$

$$[\mathrm{NO_3\,(2)}] = [\mathrm{NO_3(1)}]\frac{K_{\mathrm{L12}}}{k_{\mathrm{NO_3,2}} + K_{\mathrm{L12}}}$$

where

$$\kappa_{\mathrm{NO_3,1}} = \sqrt{D_{\mathrm{NO_3}}k_{\mathrm{NO_3,1}}}$$

$$\kappa_{\mathrm{NO_3,2}} = k_{\mathrm{NO_3,2}}H_2$$

$$\kappa^*_{\mathrm{NO_3,2}} = \left(\frac{1}{\kappa_{\mathrm{NO_3,2}}} + \frac{1}{K_{\mathrm{L12}}}\right)^{-1}$$

So that

$$\begin{aligned}
[\mathrm{NO_3(1)}] &= \frac{S[\mathrm{NO_3}] + s[\mathrm{NO_3(0)}]}{\kappa^2_{\mathrm{NO_3,1}}/s + s + \kappa^*_{\mathrm{NO_3,2}}} \\
[\mathrm{NO_3\,(2)}] &= [\mathrm{NO_3(1)}\frac{K_{\mathrm{L12}}}{\kappa_{\mathrm{NO_3,2}} + K_{\mathrm{L12}}}
\end{aligned}$$

Nitrate Source

$$\begin{aligned} S[\mathsf{NO_3}] &= J_{\mathsf{N}} + s[\mathsf{NH_4(0)}] - s[\mathsf{NH_4(1)}] \\ &= J_{\mathsf{N}} - s\Big([\mathsf{NH_4(1)}] - [\mathsf{NH_4(0)}]\Big) \\ &= J_{\mathsf{N}} - J[\mathsf{NH_4}] \end{aligned}$$

Nitrate flux

$$J[\mathsf{NO_3}] = s\Big([\mathsf{NO_3(1)}] - [\mathsf{NO_3(0)}]\Big)$$

Solution

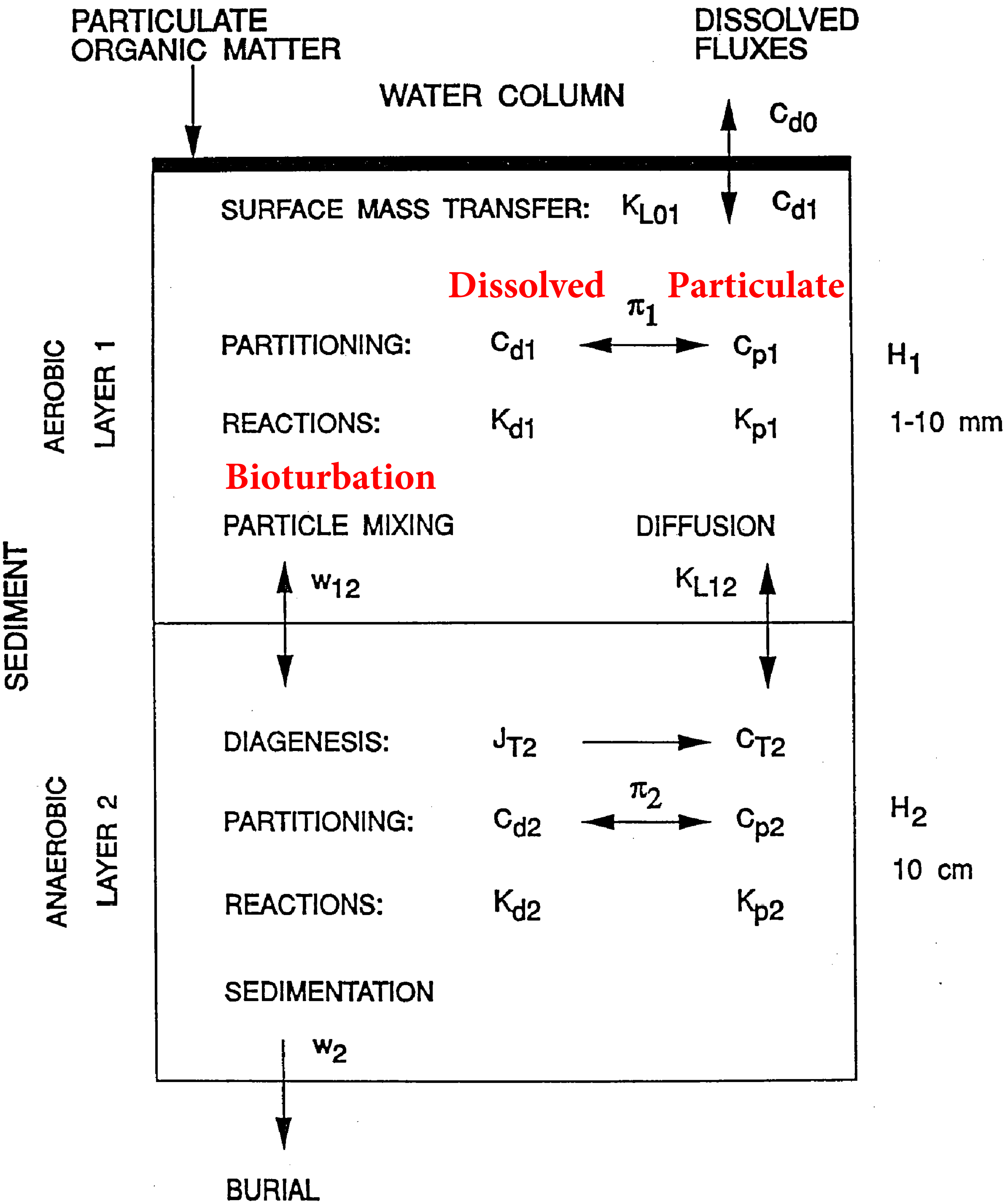
$$\begin{aligned} J[\mathsf{NO_3}] &= \left(\frac{s^2}{\kappa^2_{\mathsf{NO_3,1}}/s + s + \kappa^*_{\mathsf{NO_3,2}}} - s\right)[\mathsf{NO_3(0)}] \\ &\quad + \left(\frac{s(J_{\mathsf{N}} - J[\mathsf{NH_4}])}{\kappa^2_{\mathsf{NO_3,1}}/s + s + \kappa^*_{\mathsf{NO_3,2}}}\right) \end{aligned}$$

Two parts

1. Due to overlying water $[\mathsf{NO_3}]$

2. Due to nitrification $J_{\mathsf{N}} - J[\mathsf{NH_4}]$

SEDIMENT FLUX MODEL



Reactions

	Diagenesis	Partitioning	Reaction
NH_4	PON -> NH_4	Small	$NH_4 + O_2$ -> NO_3
NO_3			NO_3 + POC -> $N_2(g)$
H_2S	POC -> H_2S	H_2S <-> FeS(s)	$H_2S + O_2$ -> FeS + O_2 ->
PO_4	POP -> PO_4	PO_4 <-> PIP(s) $\pi_1 > \pi_2$ $\pi_1 = f[O_2(0)]$	
Si	PSi -> DSi	PSi <-> DSi	$k_{Si}P_{Si}$ (DSi - Si_{sat})
SOD			$NH_4 + O_2$ -> $H_2S + O_2$ -> FeS + O_2 ->

Transport Mechanisms

Surface Mass Transfer	Particle Mixing	Diffusion
K_{L01}	w_{12}	K_{L12}
K_{L01} = SOD / $O_2(0)$	G_1 Carbon, $O_2(0)$, T	T

Distribution Between Particulate and Dissolved Concentrations

C_d = bulk dissolved mg P / L water

C_p = bulk particulate mg P/ L water

m = particle conc. kg SS/L

q_p = particulate conc. mg P/kg SS

$q_p = C_p / m$

Partitioning Model

$q_p = K_p\ Cd$

K_p = partition coefficient (L / kg SS)

"Pie" = K_p

Sediment Bioturbation

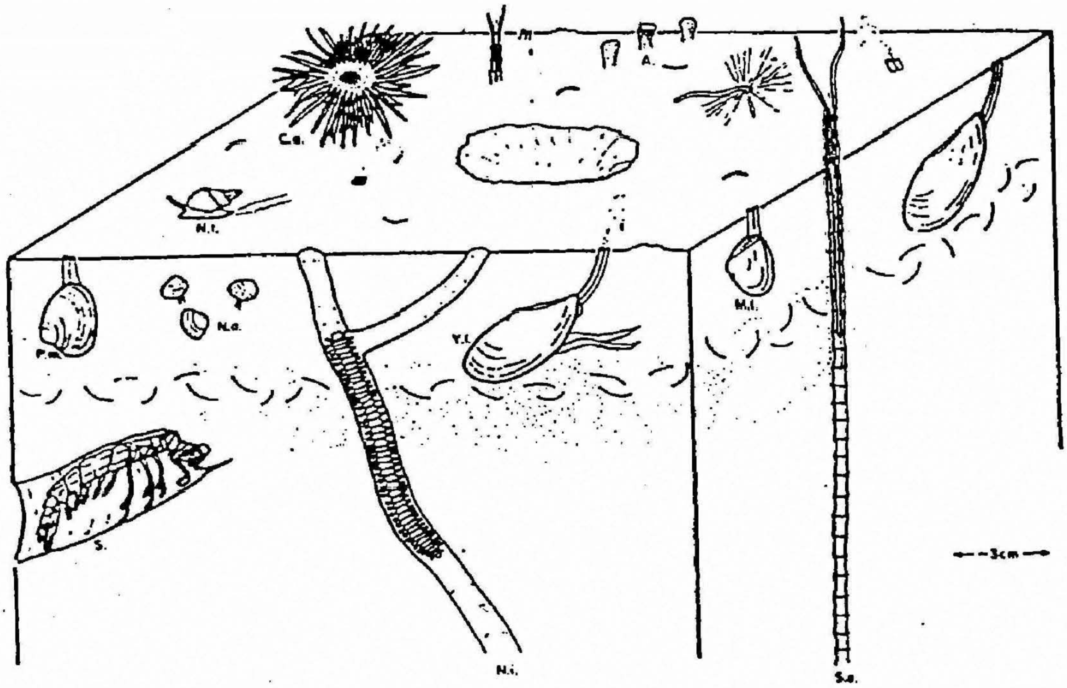
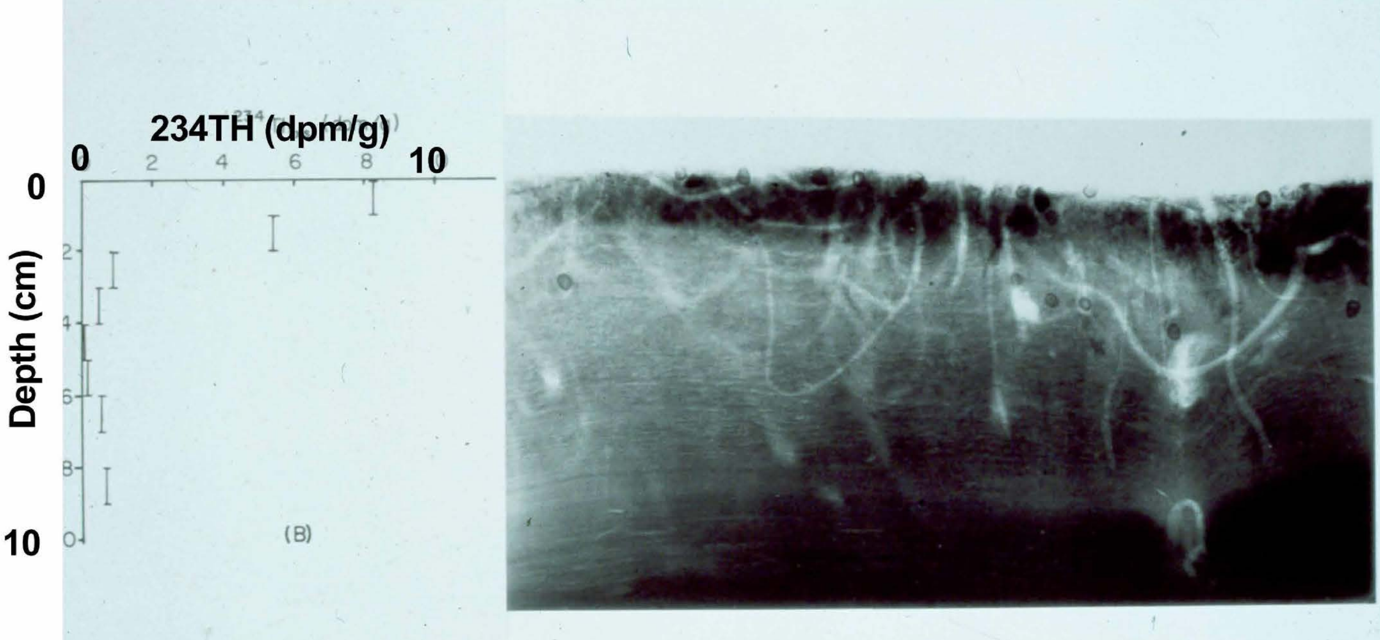
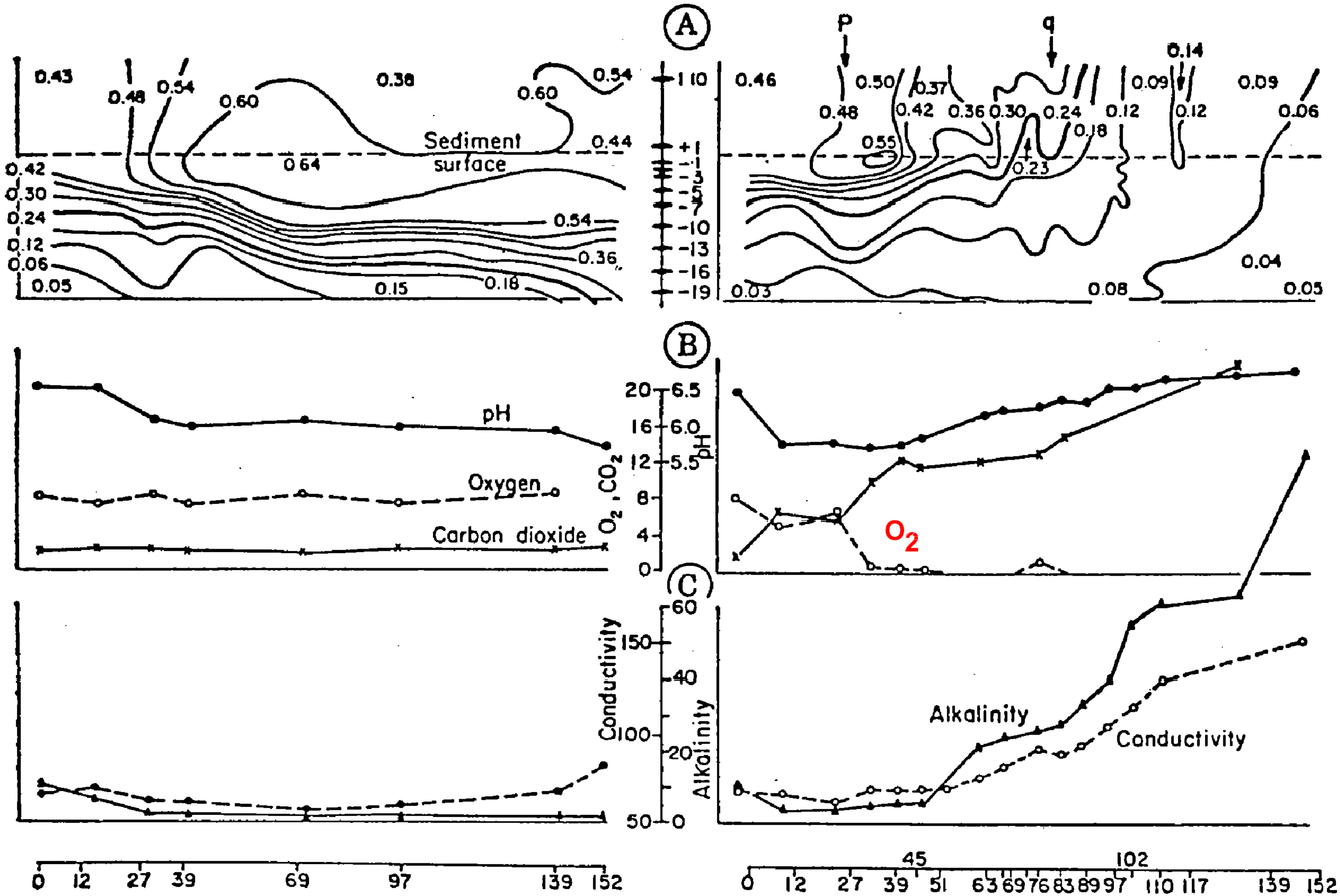


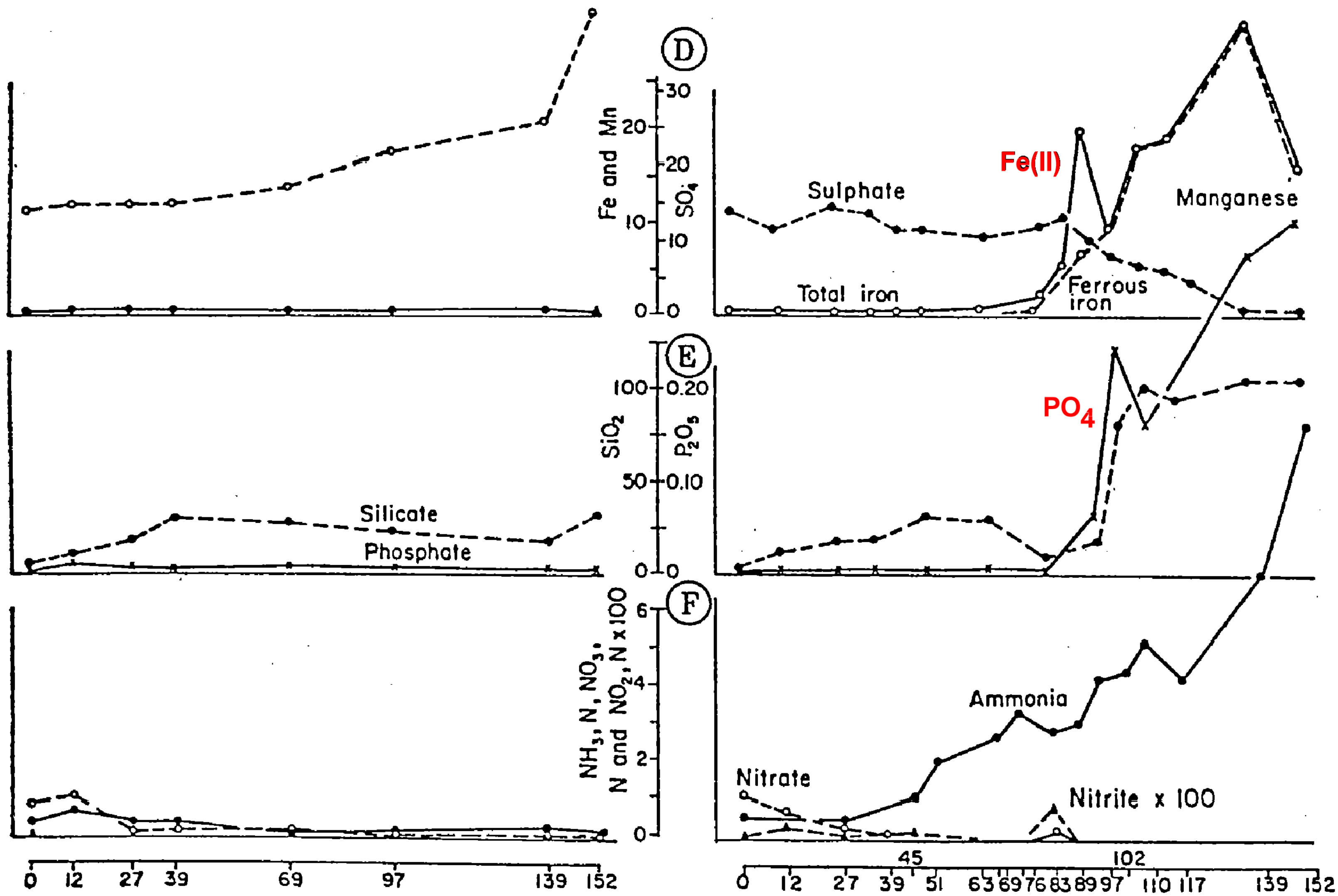
FIG. 6. Schematic drawing of major fauna at NWC: C.a., *Ceriantheopsis americanus*; P.m., *Pitar morrhuana*; and S., *Squilla*; all other abbreviations as in Fig. 3.

Aller, R.C. (1980)



Mortimer Experiments 1941-1942





D
Fe and Mn
SO_4
Fe(II)
Sulphate
Manganese
Total iron
Ferrous iron
E
SiO_2
P_2O_5
PO_4
Silicate
Phosphate
F
NH_3, N, NO_3, N and NO_2, N x 100
Ammonia
Nitrate
Nitrite x 100
0 12 27 39 69 97 139 152
0 12 27 39 45 51 63 69 76 83 89 97 102 110 117 139 152

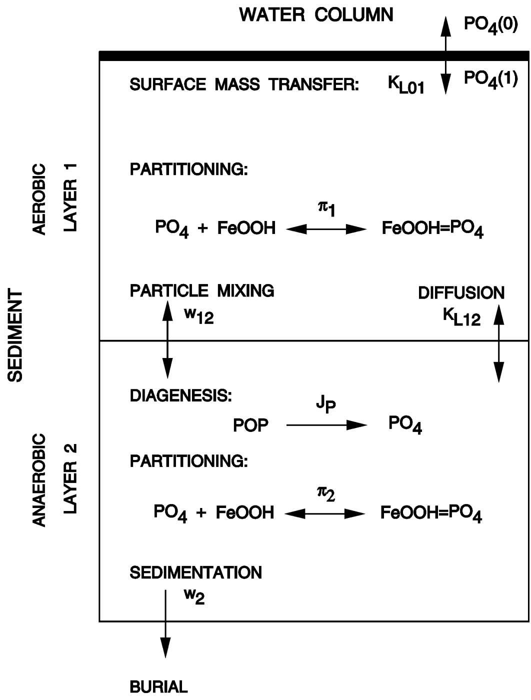


Fig. 6.1 Schematic diagram of the phosphorus flux model.

Phosphorus Flux Model

$$H_1 \frac{d[\mathrm{PO_4}(1)]_\mathrm{T}}{dt} = s\left([\mathrm{PO_4}(0)] - f_{\mathrm{d1}}[\mathrm{PO_4}(1)]_\mathrm{T}\right)$$

$$+\omega_{12}\left(f_{\mathrm{p2}}[\mathrm{PO_4}(2)]_\mathrm{T} - f_{\mathrm{p1}}[\mathrm{PO_4}(1)]_\mathrm{T}\right)$$

$$+K_{\mathrm{L12}}\left(f_{\mathrm{d2}}[\mathrm{PO_4}(2)]_\mathrm{T} - f_{\mathrm{d1}}[\mathrm{PO_4}(1)]_\mathrm{T}\right)$$

$$-\omega_2[\mathrm{PO_4}(1)]_\mathrm{T} \qquad (6.1a)$$

$$H_2 \frac{d[\mathrm{PO_4}(2)]_\mathrm{T}}{dt} = -\omega_{12}\left(f_{\mathrm{p2}}[\mathrm{PO_4}(2)]_\mathrm{T} - f_{\mathrm{p1}}[\mathrm{PO_4}(1)]_\mathrm{T}\right)$$

$$-K_{\mathrm{L12}}\left(f_{\mathrm{d2}}[\mathrm{PO_4}(2)]_\mathrm{T} - f_{\mathrm{d1}}[\mathrm{PO_4}(1)]_\mathrm{T}\right)$$

$$+\omega_2\left([\mathrm{PO_4}(1)]_\mathrm{T} - [\mathrm{PO_4}(2)]_\mathrm{T}\right) + J_\mathrm{P} \qquad (6.1b)$$

where

H_1 and H_2 are the depths of the aerobic (1) and anaerobic (2) layers

$[PO_4(0)]$ is the dissolved phosphate concentration in the overlying water

$[PO_4(1)]_T$ and $[PO_4(2)]_T$ are the total phosphate concentrations in layers 1 and 2

f_{d1}, and f_{d2} are the dissolved fractions in layers 1 and 2

f_{p1} and f_{p2} are the particulate fractions in layers 1 and 2

s is the surface mass transfer coefficient between the overlying water and the aerobic layer

K_{L12} is the mass transfer coefficient between the aerobic and anaerobic layers

w_{12} is the particle mixing velocity between the aerobic and anaerobic layers

w_2 is the burial velocity

J_P is the source of phosphate from the diagenesis of particulate organic phosphorus POP

$$J[PO_4] \approx J_P \frac{s f_{d1}}{s f_{d1} + w_2 \left(\frac{K_{L12} f_{d1} + s f_{d1}}{K_{L12} f_{d2}} \right)} = \frac{s}{s + w_2 \left(\frac{K_{L12} + s}{K_{L12} f_{d2}} \right)}$$

The dissolved f_d and particulate f_p fractions are computed from the partitioning equations

$$f_d = \frac{\phi}{1 + m_1\pi_1/\phi} \tag{5.2a}$$

$$f_p = \frac{m_1\pi_1/\phi}{1 + m_1\pi_1/\phi} \tag{5.2b}$$

where the solids concentrations are m_1 and m_2, and the partition coefficients are π_1 and π_2, respectively. Note that the solids concentration partition coefficient products: $m_1\pi_1$ and $m_2\pi_2$ determine the extent of partitioning. The concentrations of dissolved and particulate chemical are obtained as products of these fractions and the total concentrations C_{T1} and C_{T2}.

$$\pi_1 = \pi_2(\Delta\pi_{PO_4,1}) \qquad [O_2(0)] > [O_2(0)]_{crit,PO_4} \tag{6.19}$$

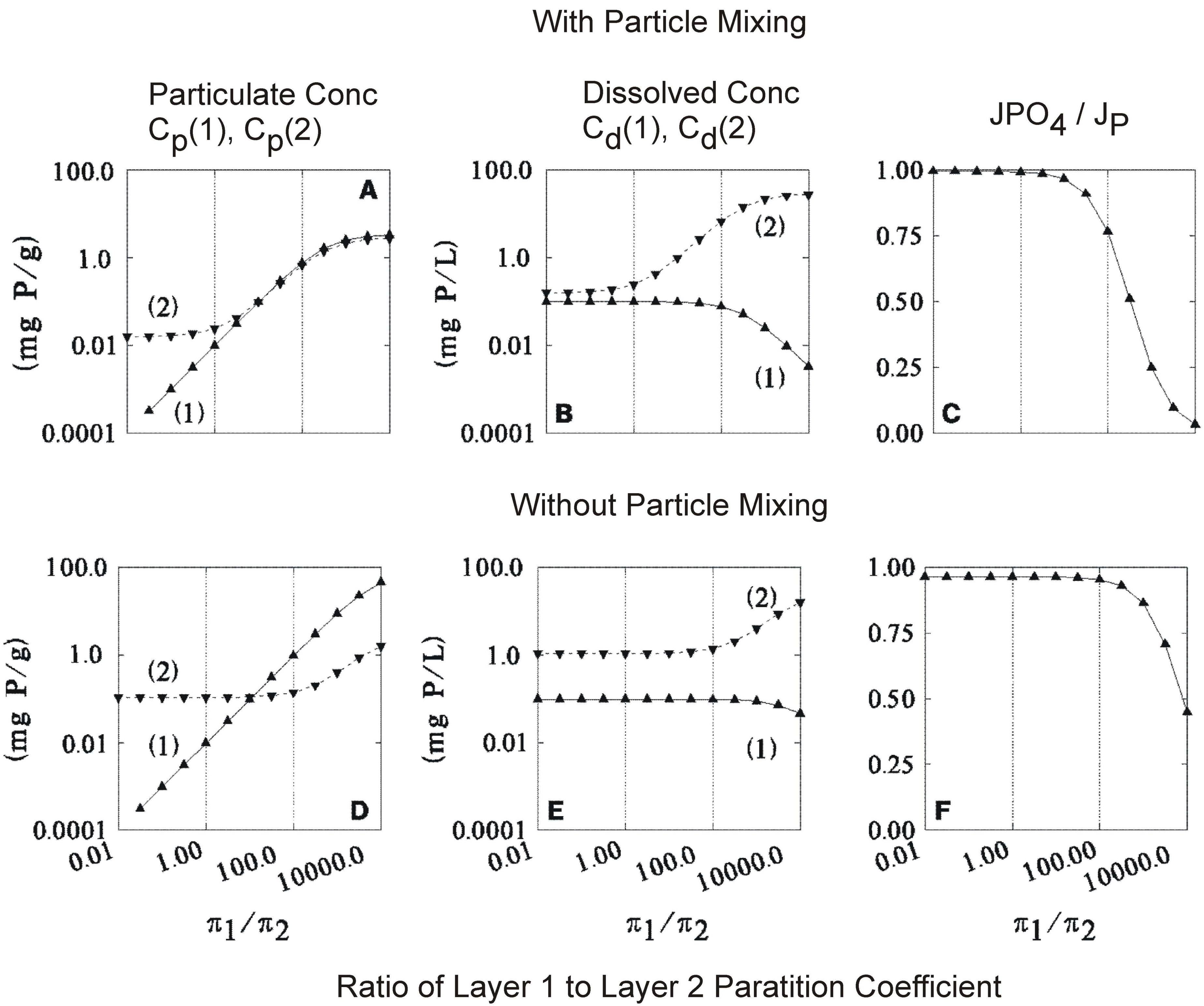
However, if oxygen falls below a critical concentration, $[O_2(0)] < [O_2(0)]_{crit,PO_4}$, then

$$\pi_1 = \pi_2(\Delta\pi_{PO_4,1})^{\beta_{PO_4}} \qquad [O_2(0)] \leqslant [O_2(0)]_{crit,PO_4} \tag{6.20}$$

where

$$\beta_{PO_4} = \frac{[O_2(0)]}{[O_2(0)]_{crit,PO_4}} \tag{6.21}$$

Eq. (6.20) smoothly reduces the aerobic layer partition coefficient to that in the anaerobic layer as $[O_2(0)]$ goes to zero.



With Particle Mixing
Particulate Conc
Cp(1), Cp(2)
Dissolved Conc
Cd(1), Cd(2)
JPO4 / JP
A
B
C
(1)
(2)
(mg P/g)
(mg P/L)
100.0
1.0
0.01
0.0001
1.00
0.75
0.50
0.25
0.00
Without Particle Mixing
D
E
F
0.01
1.00
100.0
100.00
10000.0
π1/π2
Ratio of Layer 1 to Layer 2 Paratition Coefficient

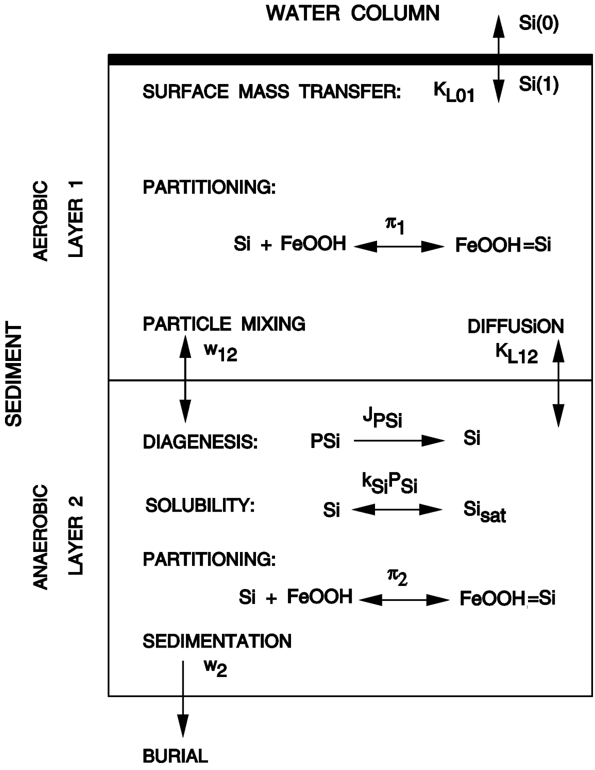


Fig. 7.1 Schematic diagram of the silica flux model.

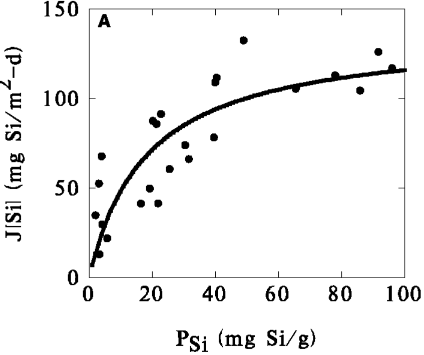


Fig. 7.3 (A) Silica flux versus particulate silica
tration versus distance along the axis of Chesape

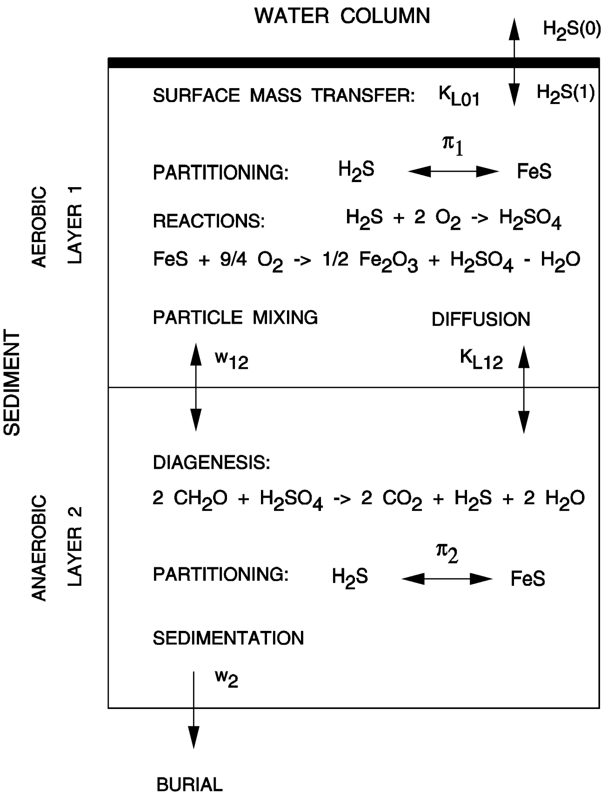


Fig. 9.1 Schematic diagram of the sulfide oxidation model.

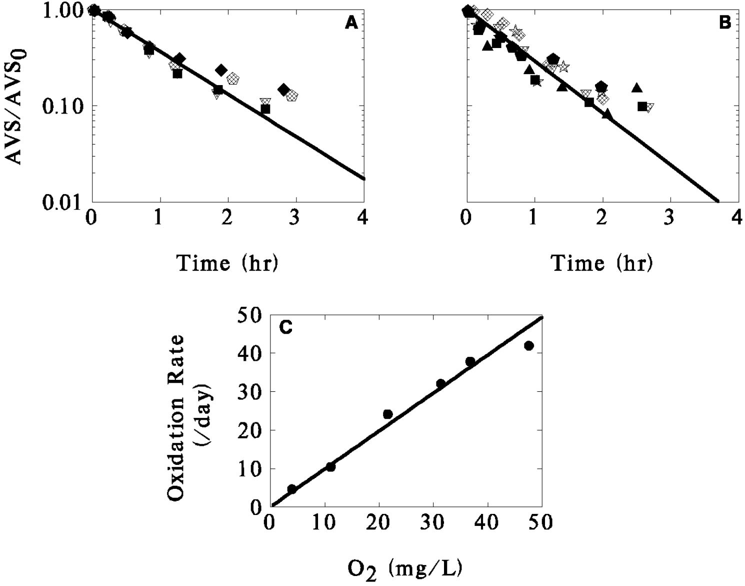


Fig. 9.2 Kinetics of FeS(s) oxidation for (A) Jamacia Bay and (B) Van Cortlandt Pond sediments (Di Toro et al., 1996a). (C) Effect of dissolved oxygen concentration on the oxidation rate (Nelson, 1978).

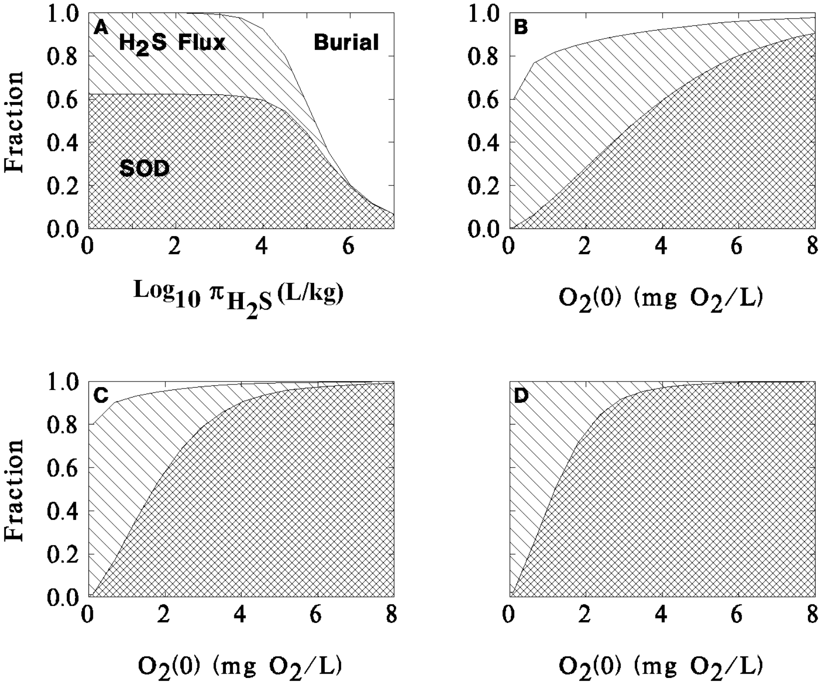


Fig. 9.3 (A) Effect of partition coefficients and (B) overlying water dissolved oxygen with increasing particulate sulfide oxidation rate (C-D) on the fraction of J_C that is oxidized as SOD J_{ox}, diffuses to the overlying water as an H_2S flux J_{aq}, or is buried J_{br}. See Table 9.1 for parameter values.

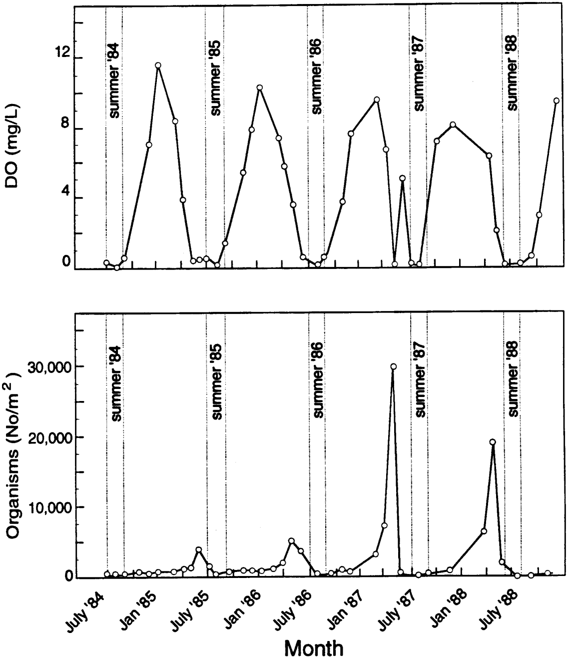


Fig. 13.4 Benthic organism density and bottom water dissolved oxygen for a deep water station in Chesapeake Bay. Data from Versar (1990).

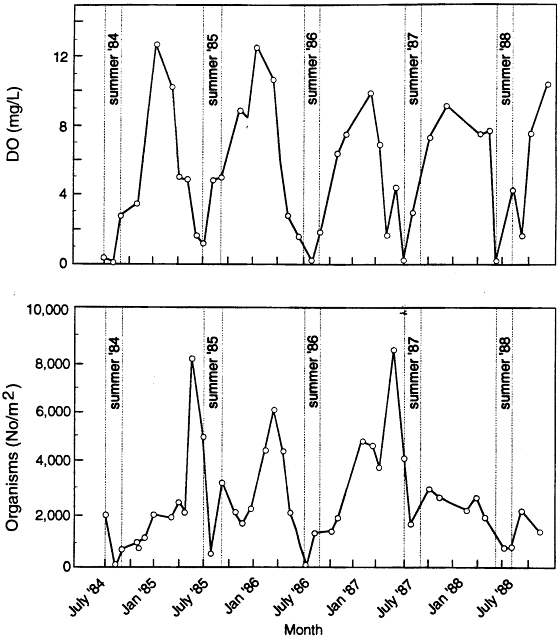
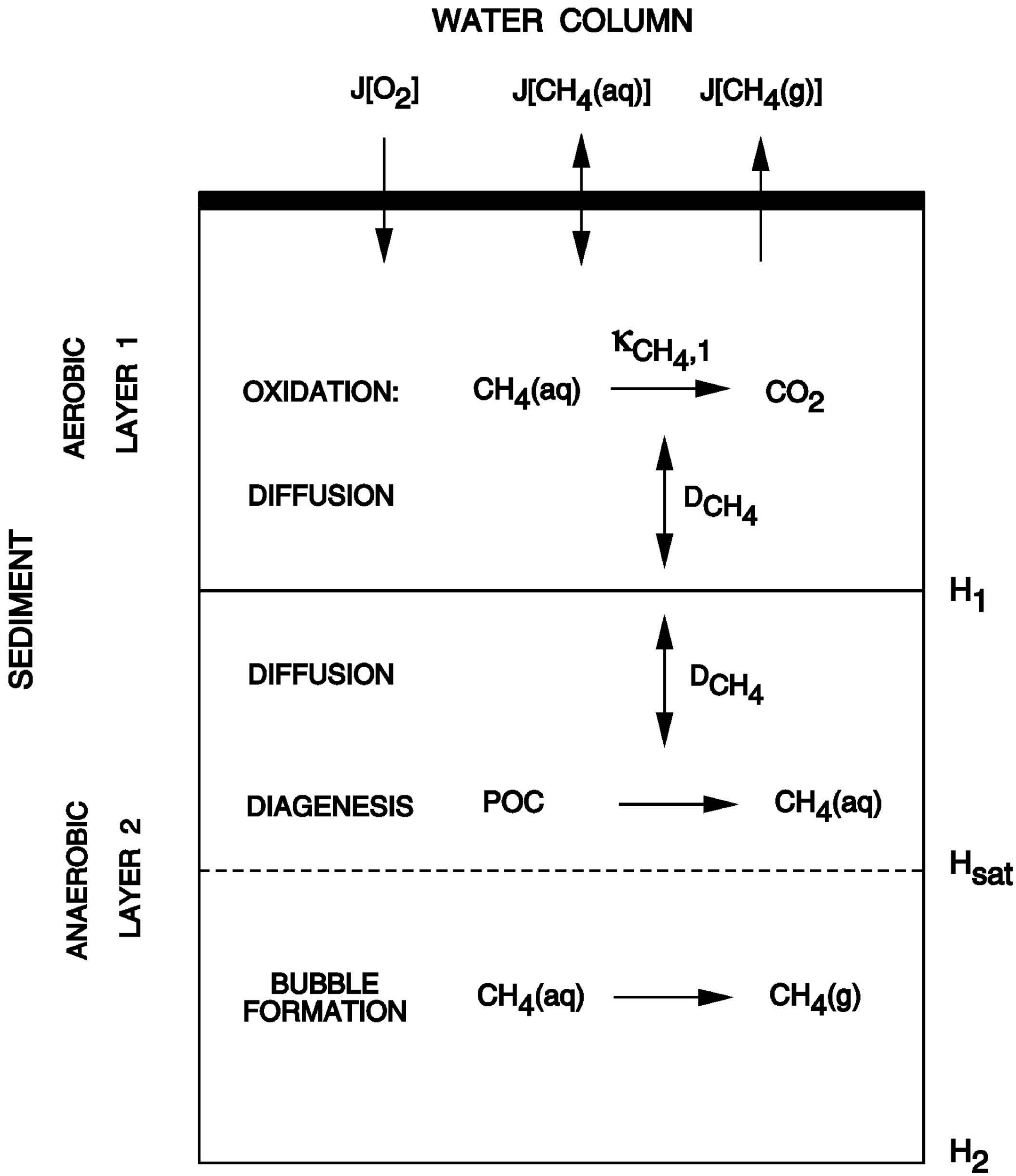


Fig. 13.5 Benthic organism density and bottom water dissolved oxygen for a station near the deep trough in Chesapeake Bay. Data from Versar (1990).

Methane Model



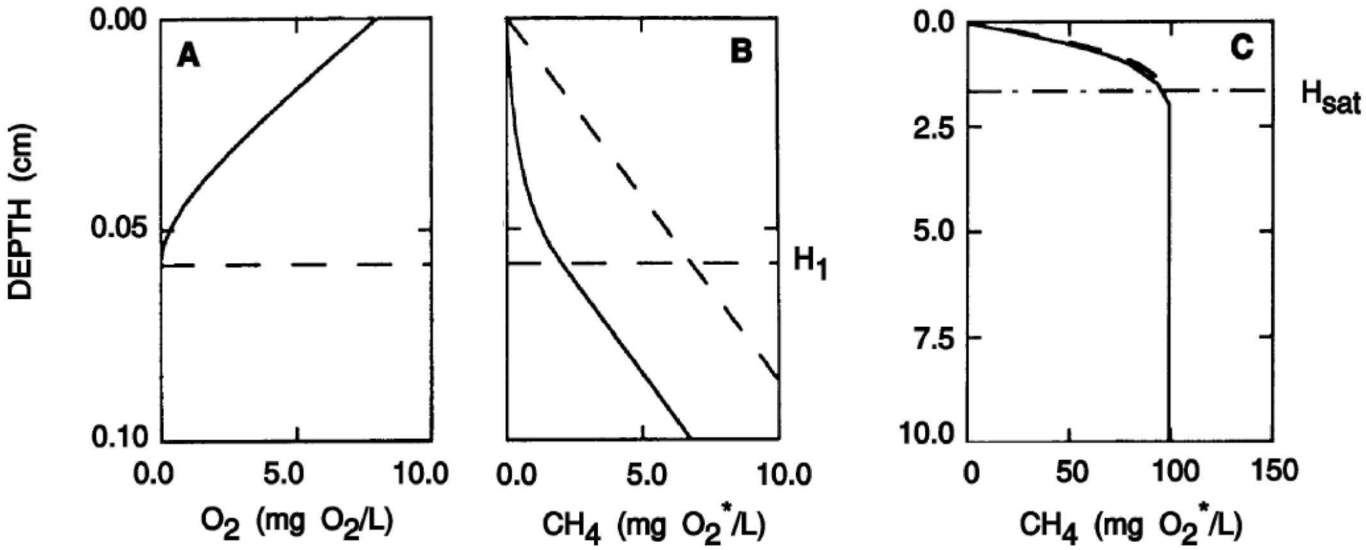


Fig. 10.2 Interstitial water concentrations profiles of dissolved oxygen and methane versus depth. (A) $O_2(z)$ from $z = 0$ to $z = 1$ mm. (B) $CH_4(aq)$ from $z = 0$ to $z = 1$ mm. (C) $CH_4(aq)$ from $z = 0$ to $z = 10$ cm. Dashed lines are for $\kappa_{CH_4,1} = 0$. Aerobic zone depth H_1 and depth of methane saturation H_{sat} are shown. Parameter values are given in Table 10.1.

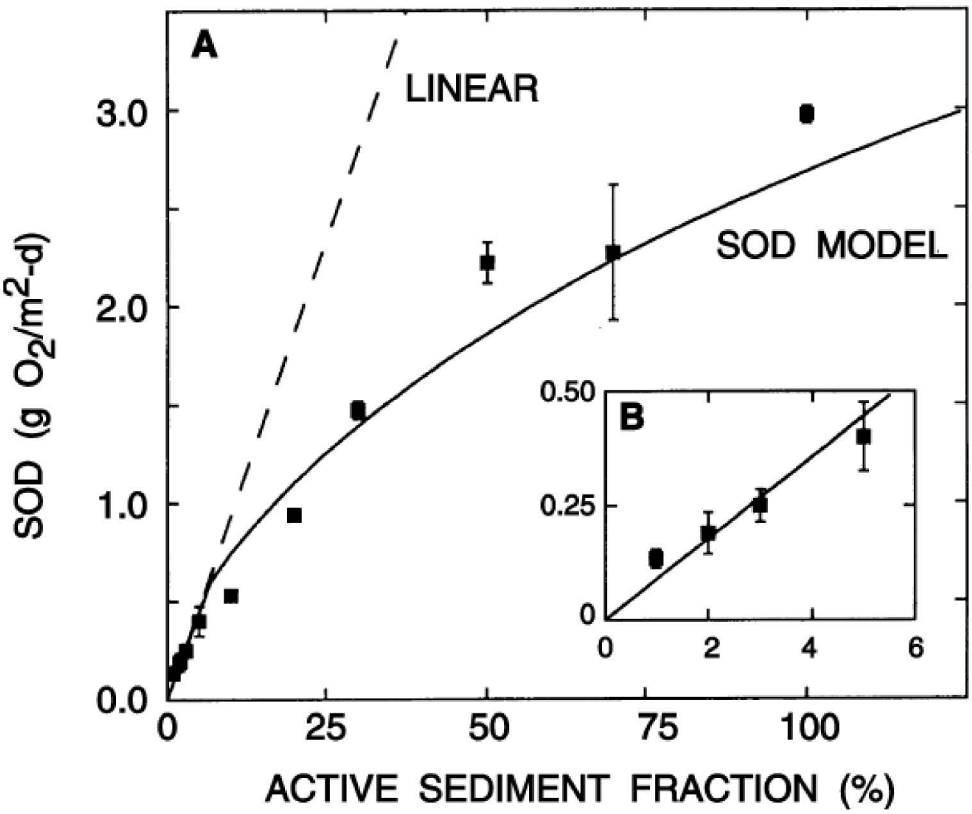


Fig. 10.3 Sediment dilution experiment. SOD versus percent of Milwaukee River sediment in the mixture. Data (mean ± standard deviation). SOD model (solid lines computed using Eqs. (10.43). Parameters are listed in Table 10.3. Axes and labels for the inset Fig. B are the same as (A). Dashed line in (A) is an extrapolation of the linear portion of the model result, shown in the inset figure (B).

SOD and Ammonia Flux vs Gas Flux

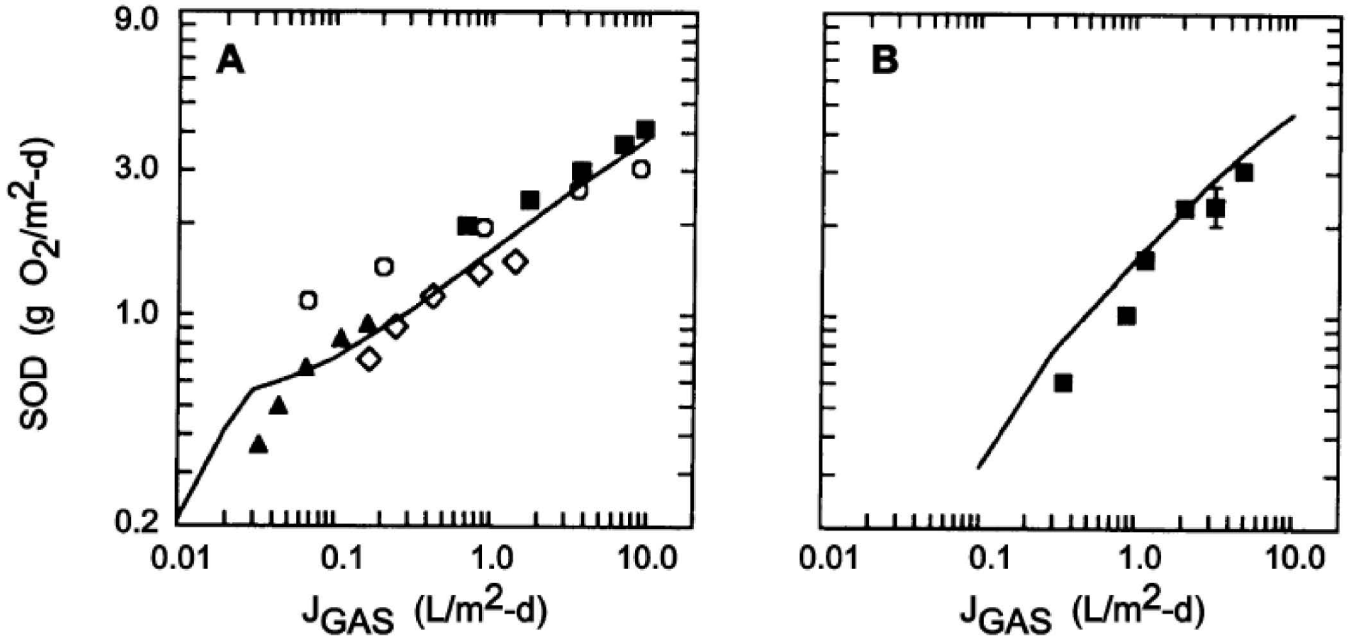


Fig. 10.4 SOD versus total gas flux. (A) Fair et al. (1941) Reactor depth (cm) = 1.42(▲), 2.55(■), 4.75(□), 10.2(◇). (B) Sediment dilution experiment. Lines are computed using Eqs. (10.43, 10.55, 10.56). Parameter values given in Table 10.3.

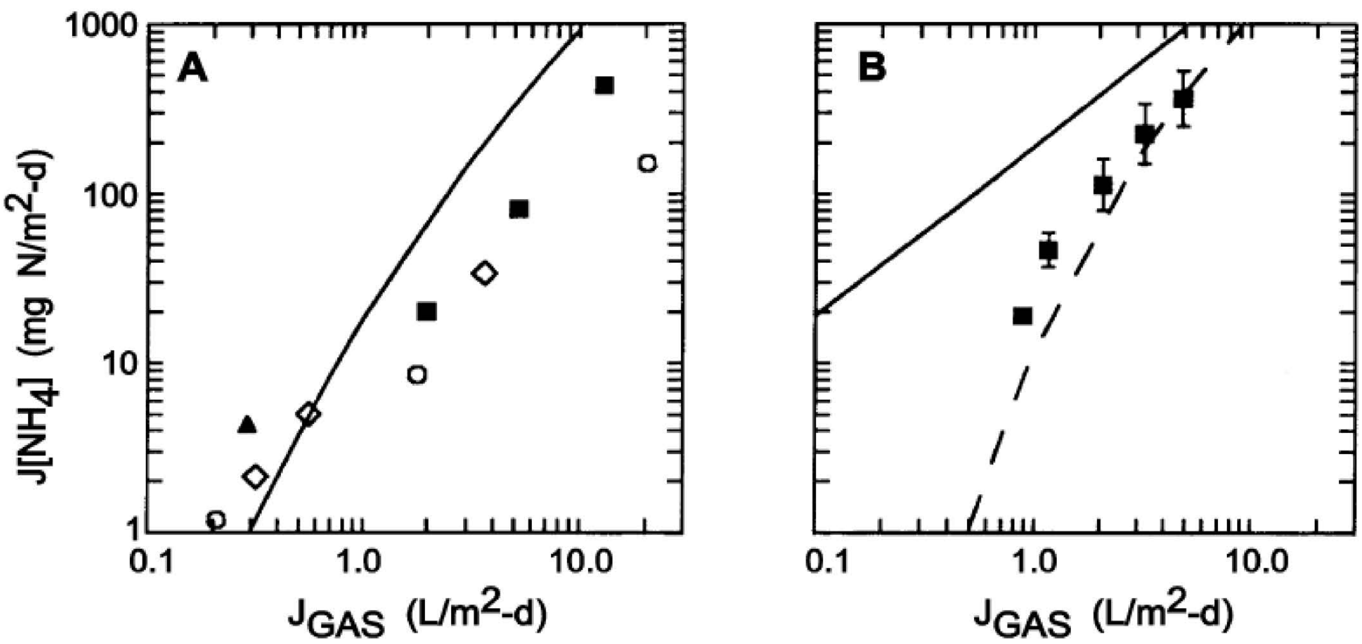


Fig. 10.5 Ammonia flux versus total gas flux. (A) Fair et al. (1941) data. Reactor depth (cm) = 1.42(▲), 2.55(■), 4.75(□), 10.2(◇). (B) Sediment dilution experiment. Anaerobic (solid line) and aerobic (dashed line) flux. Lines are computed using Eqs. (10.43a, 10.55, 10.56). Parameter values given in Table 10.3.

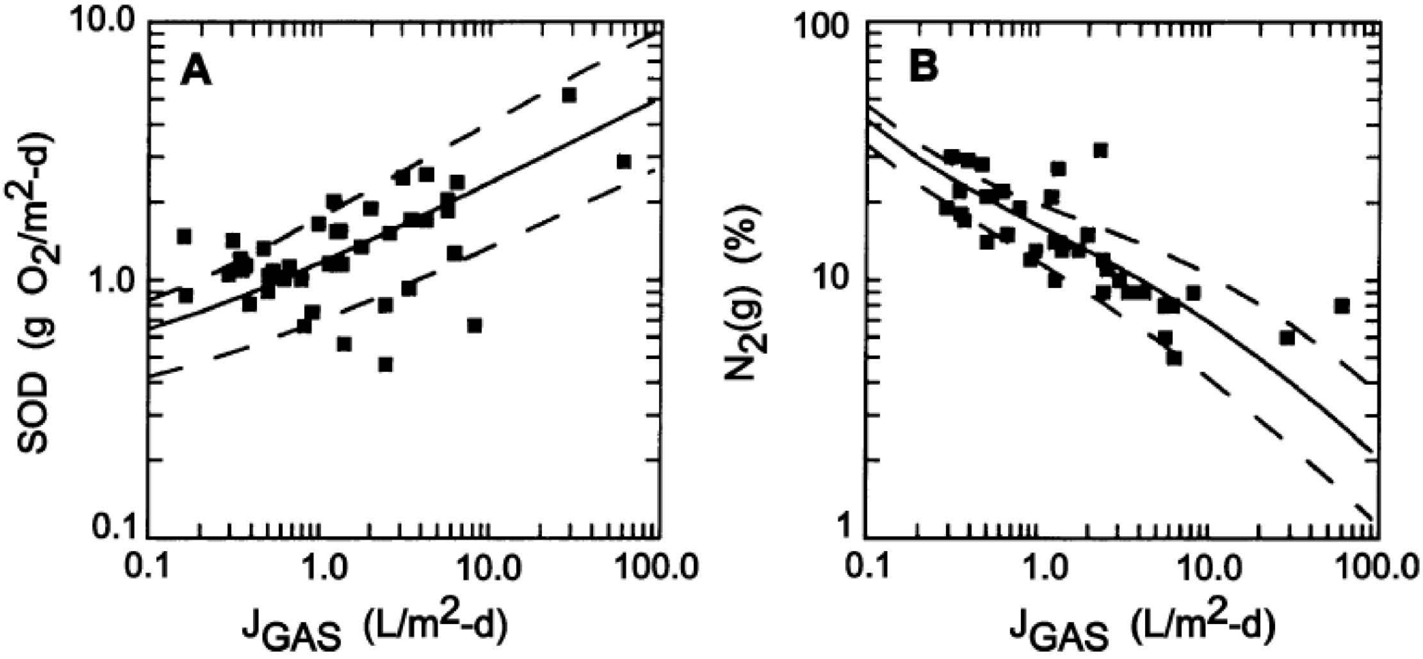
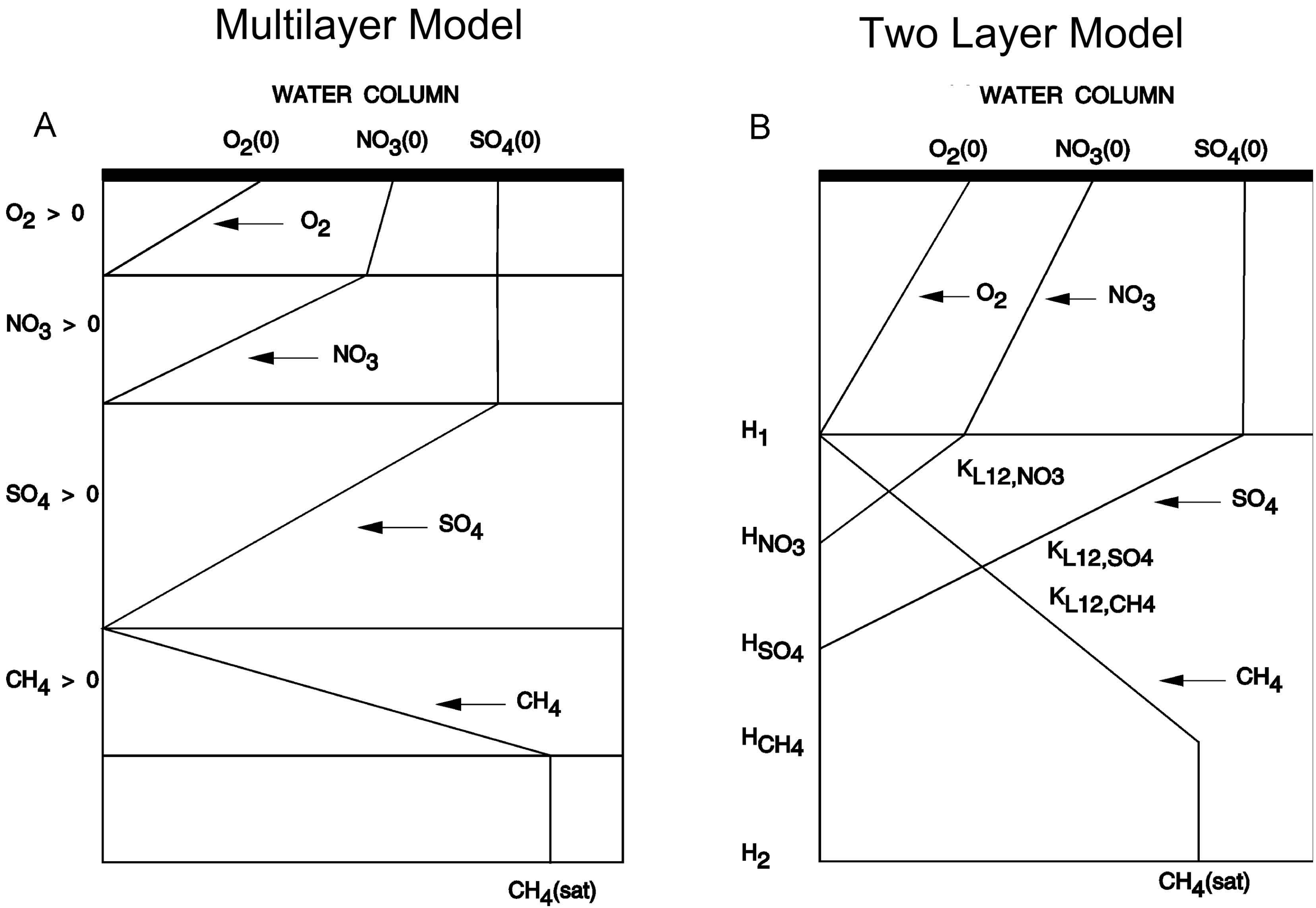


Fig. 10.6 Milwaukee River (A) SOD and (B) percent nitrogen gas versus total gas flux. Lines are computed using Eqs. (10.43, 10.55−10.56). Parameter values given in Table 10.3. Model results are evaluated using the median (solid) and the median plus and minus the standard deviation (dashed) of DO, temperature, and methane saturation concentration, given in Table 10.4.


Multilayer Model
WATER COLUMN
A
O2(0)
NO3(0)
SO4(0)
O2 > 0
O2
NO3 > 0
NO3
SO4 > 0
SO4
CH4 > 0
CH4
CH4(sat)
Two Layer Model
WATER COLUMN
B
O2(0)
NO3(0)
SO4(0)
O2
NO3
H1
KL12,NO3
HNO3
SO4
KL12,SO4
KL12,CH4
HSO4
CH4
HCH4
H2
CH4(sat)

Example Computations

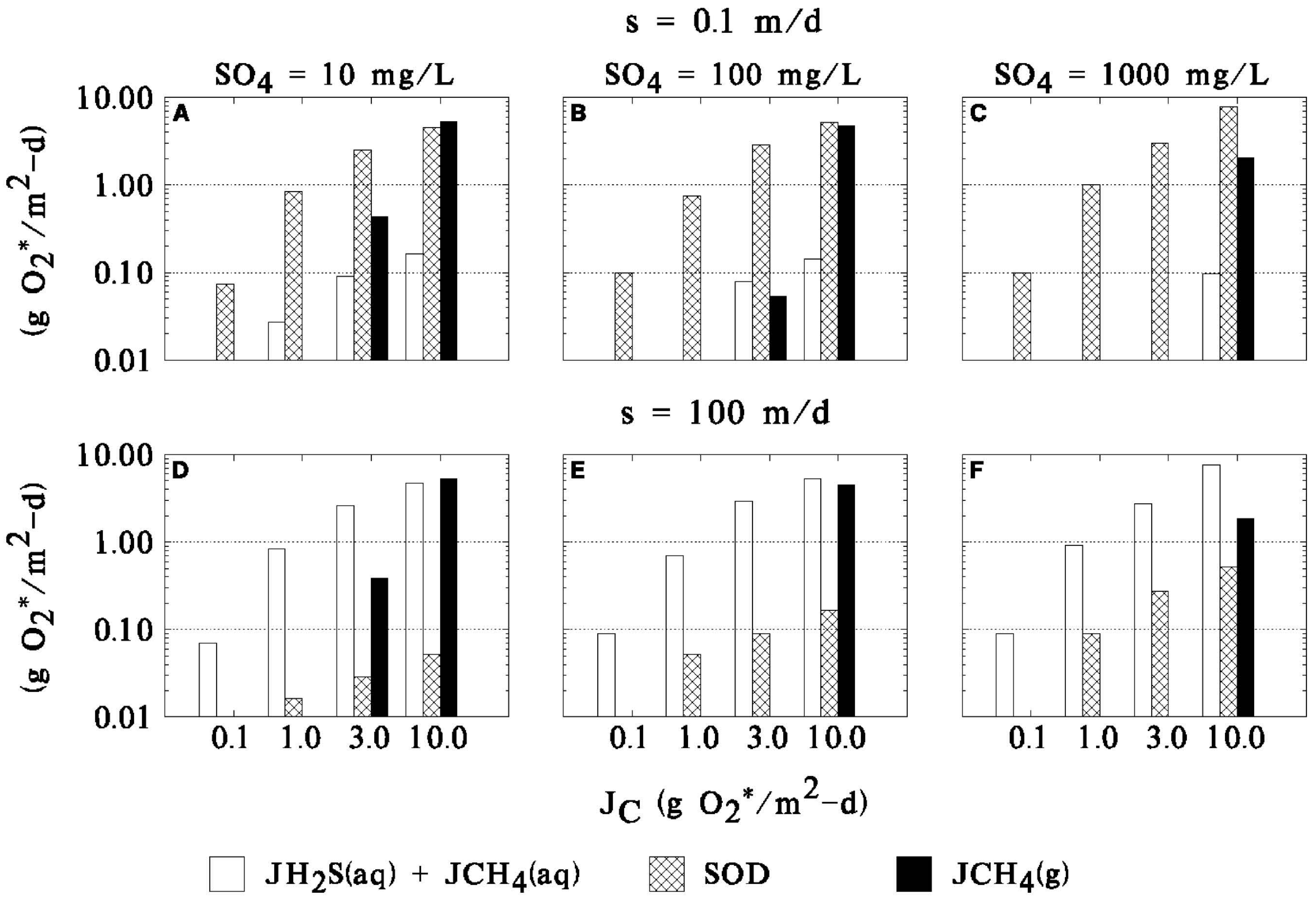
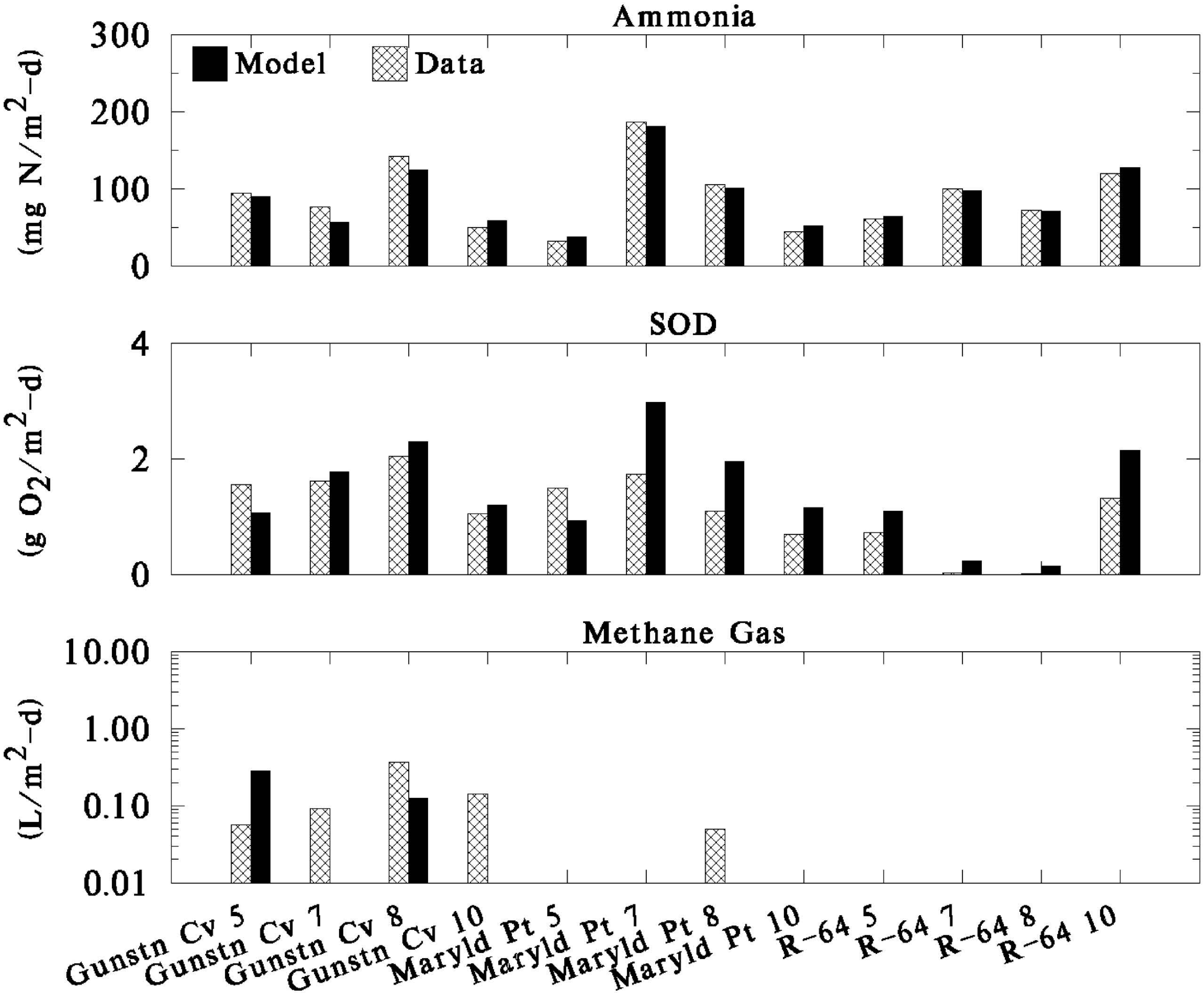
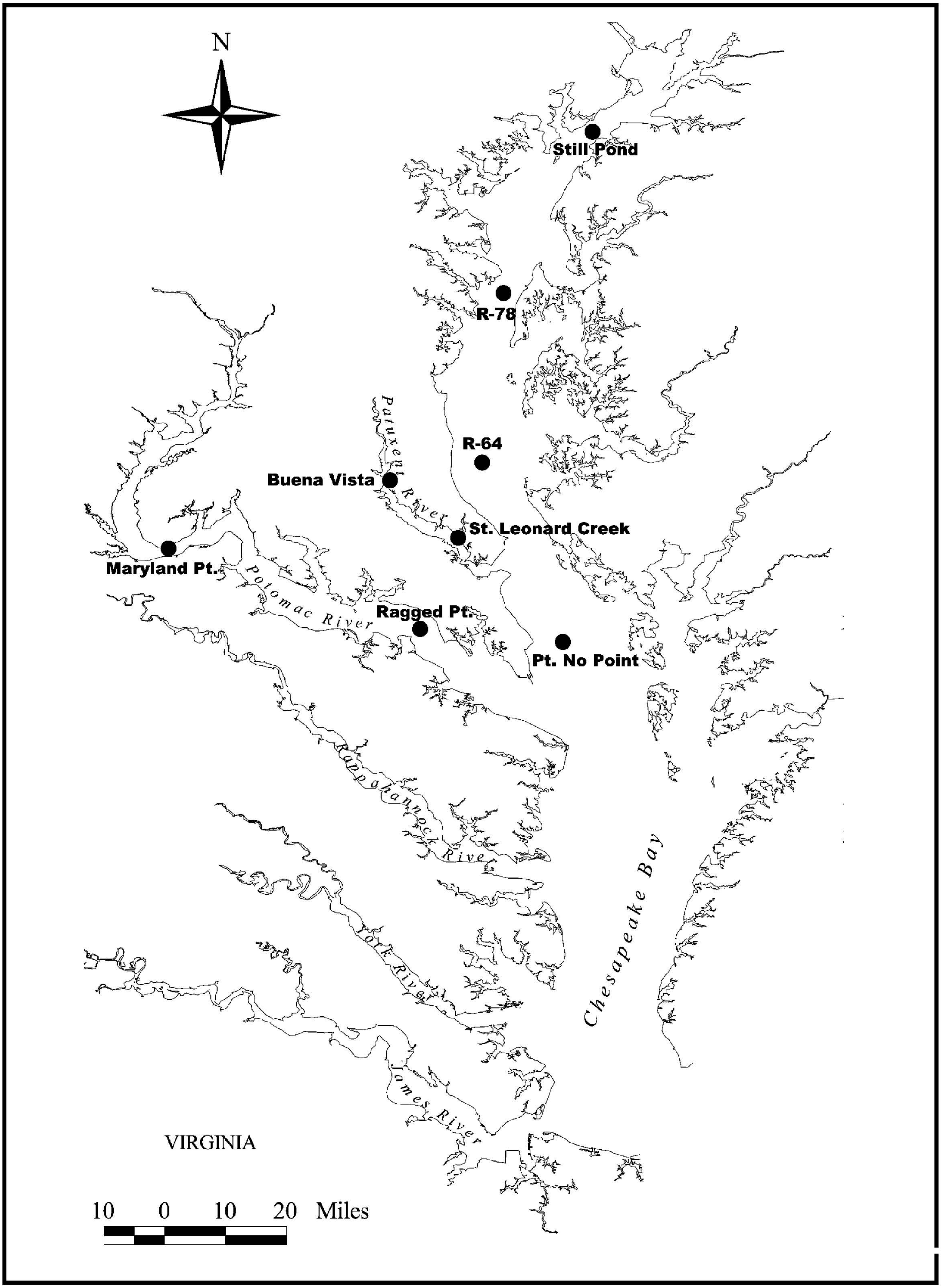


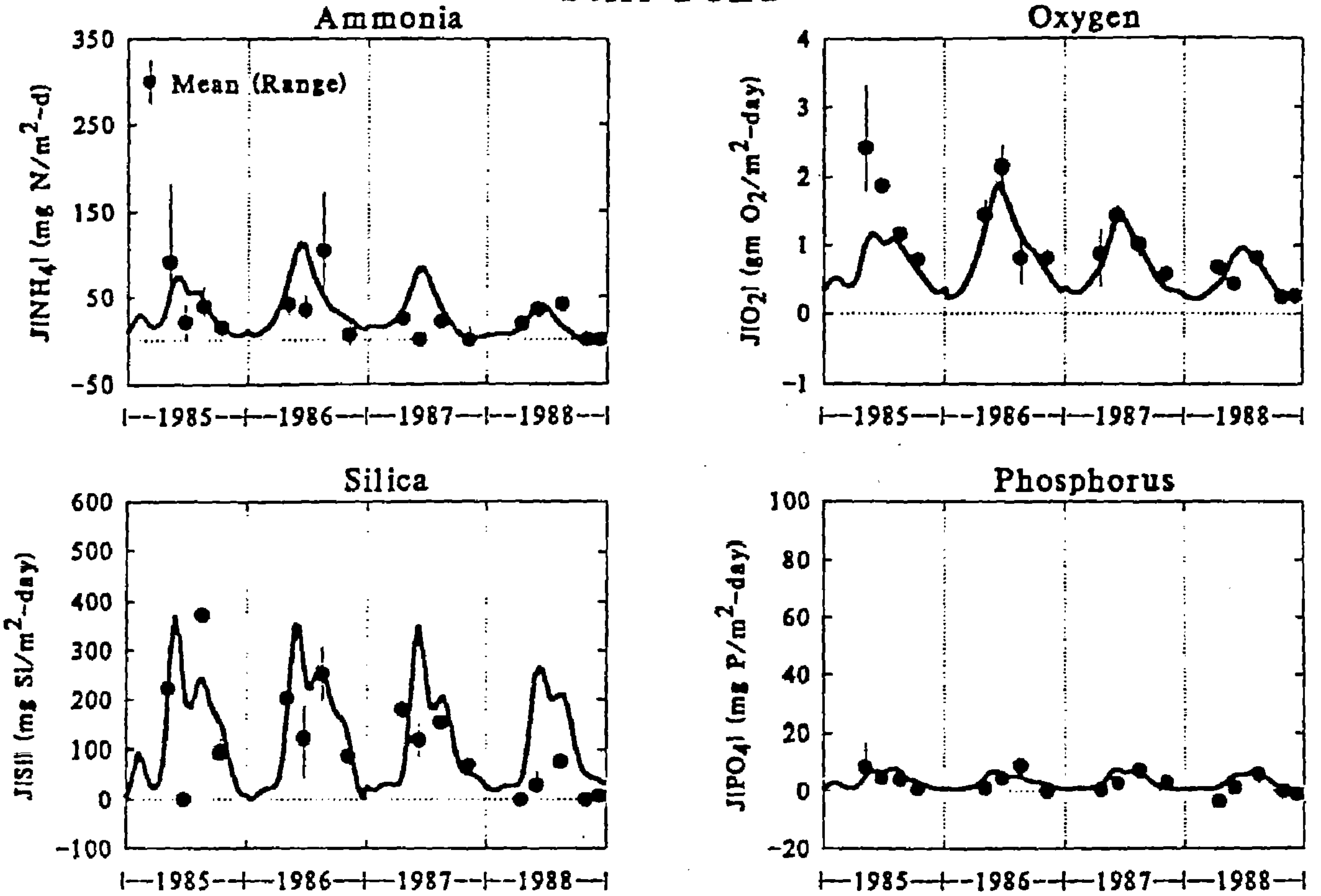
Fig. 11.7 Computed SOD, sulfide, and methane flux as a function of the surface mass transfer coefficient *s* (top and bottom rows), overlying water sulfate concentration [$SO_4(0)$] (the three columns), and carbon diagenesis J_C (abscissa).

Model - Data Comparisons

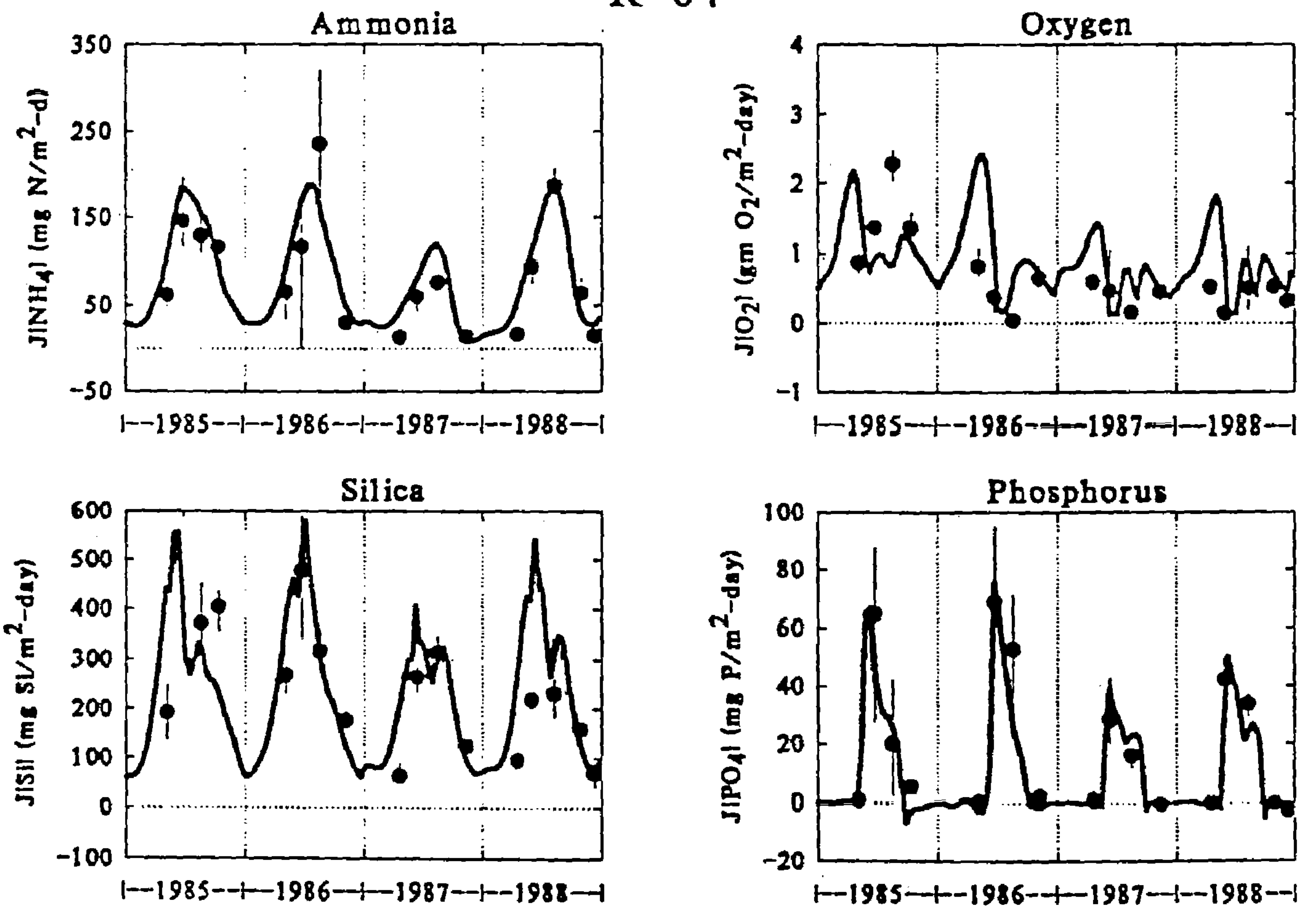


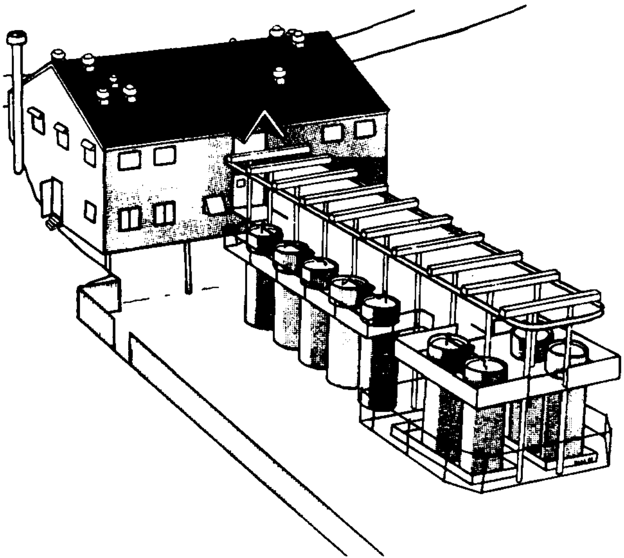

N
Still Pond
R-78
R-64
Buena Vista
Patuxent River
St. Leonard Creek
Maryland Pt.
Potomac River
Ragged Pt.
Pt. No Point
Rappahannock River
Chesapeake Bay
York River
James River
VIRGINIA
10 0 10 20 Miles

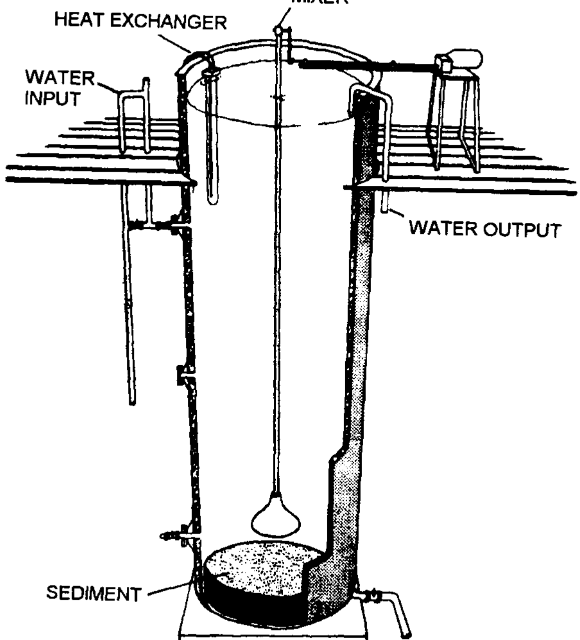
Still Pond

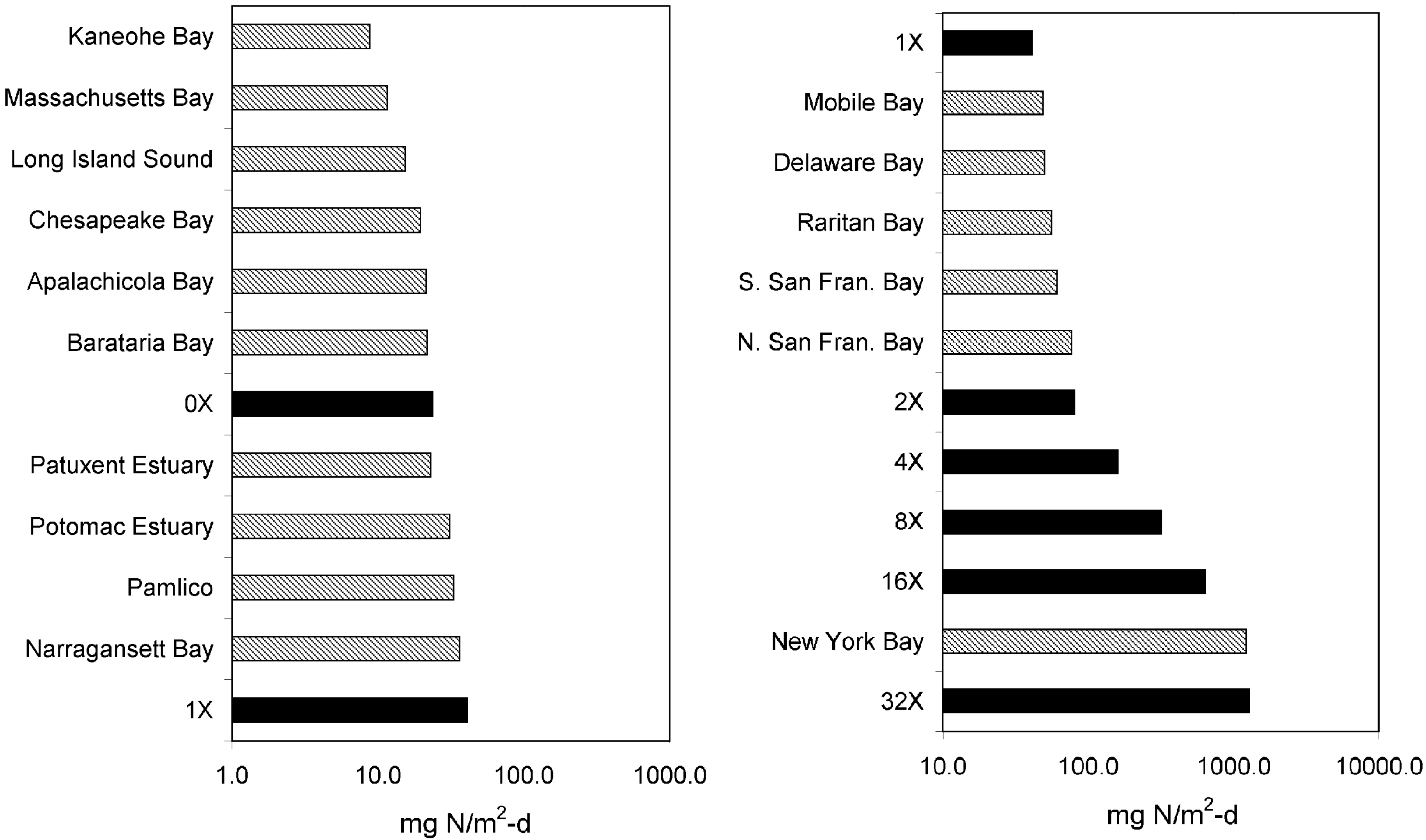


R-64



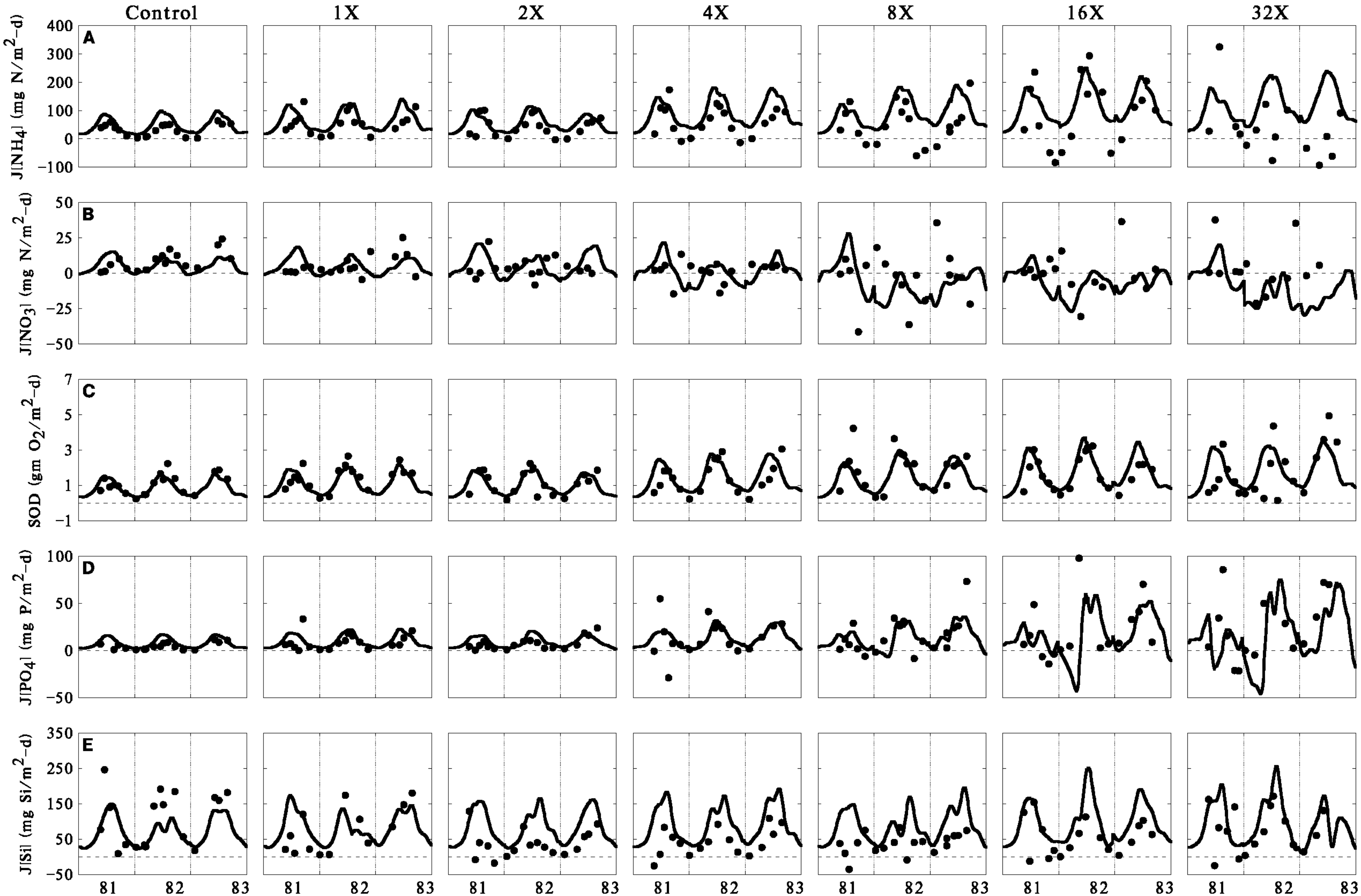



MIXER
HEAT EXCHANGER
WATER INPUT
WATER OUTPUT
SEDIMENT



Kaneohe Bay
Massachusetts Bay
Long Island Sound
Chesapeake Bay
Apalachicola Bay
Barataria Bay
0X
Patuxent Estuary
Potomac Estuary
Pamlico
Narragansett Bay
1X
1.0
10.0
100.0
1000.0
mg N/m2-d
1X
Mobile Bay
Delaware Bay
Raritan Bay
S. San Fran. Bay
N. San Fran. Bay
2X
4X
8X
16X
New York Bay
32X
10.0
100.0
1000.0
10000.0
mg N/m2-d

Sediment Flux Model Validation (MERL Mesocosm)



Di Toro, D. M. (2001).

Chesapeake Bay Ammonia Flux Calibration

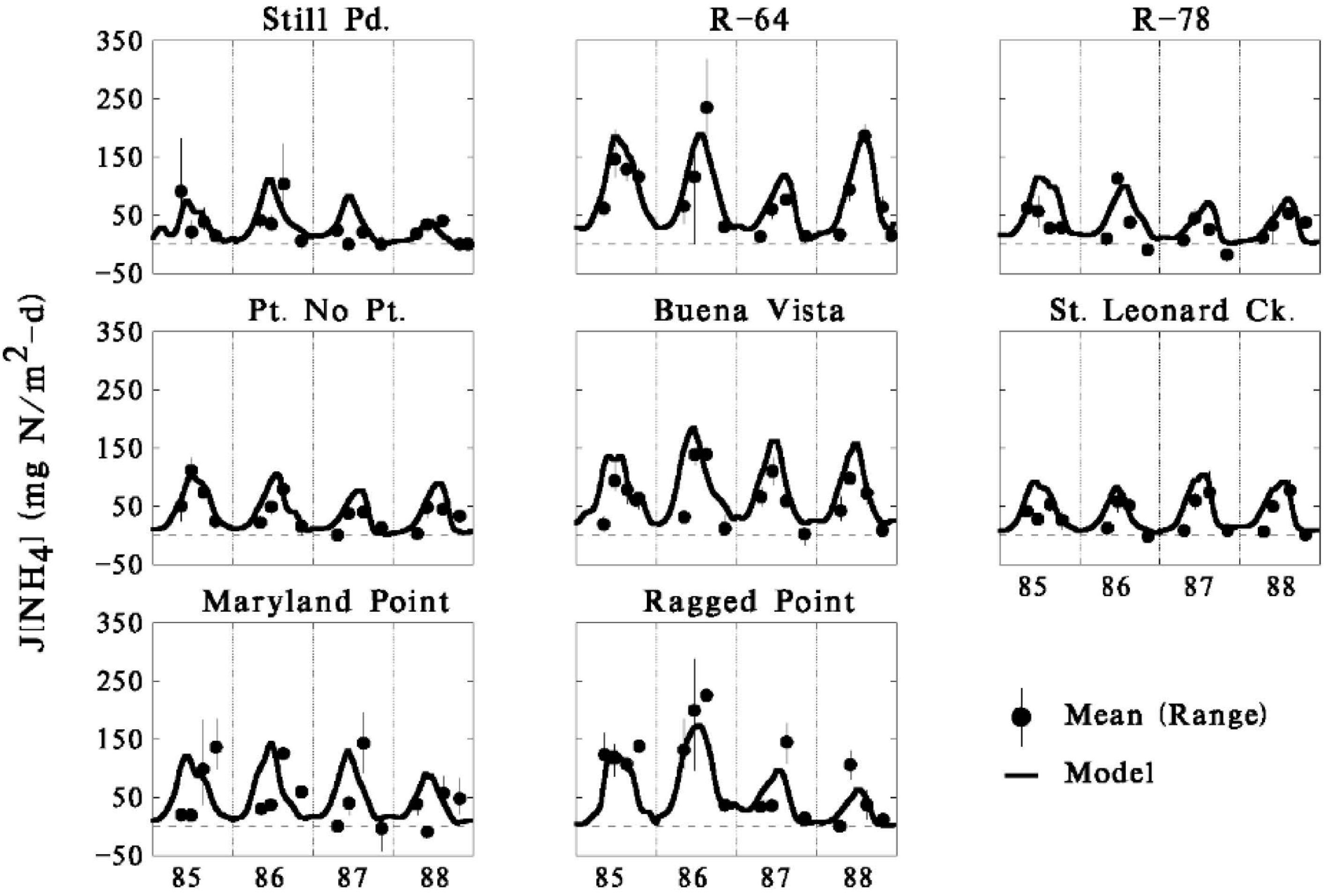
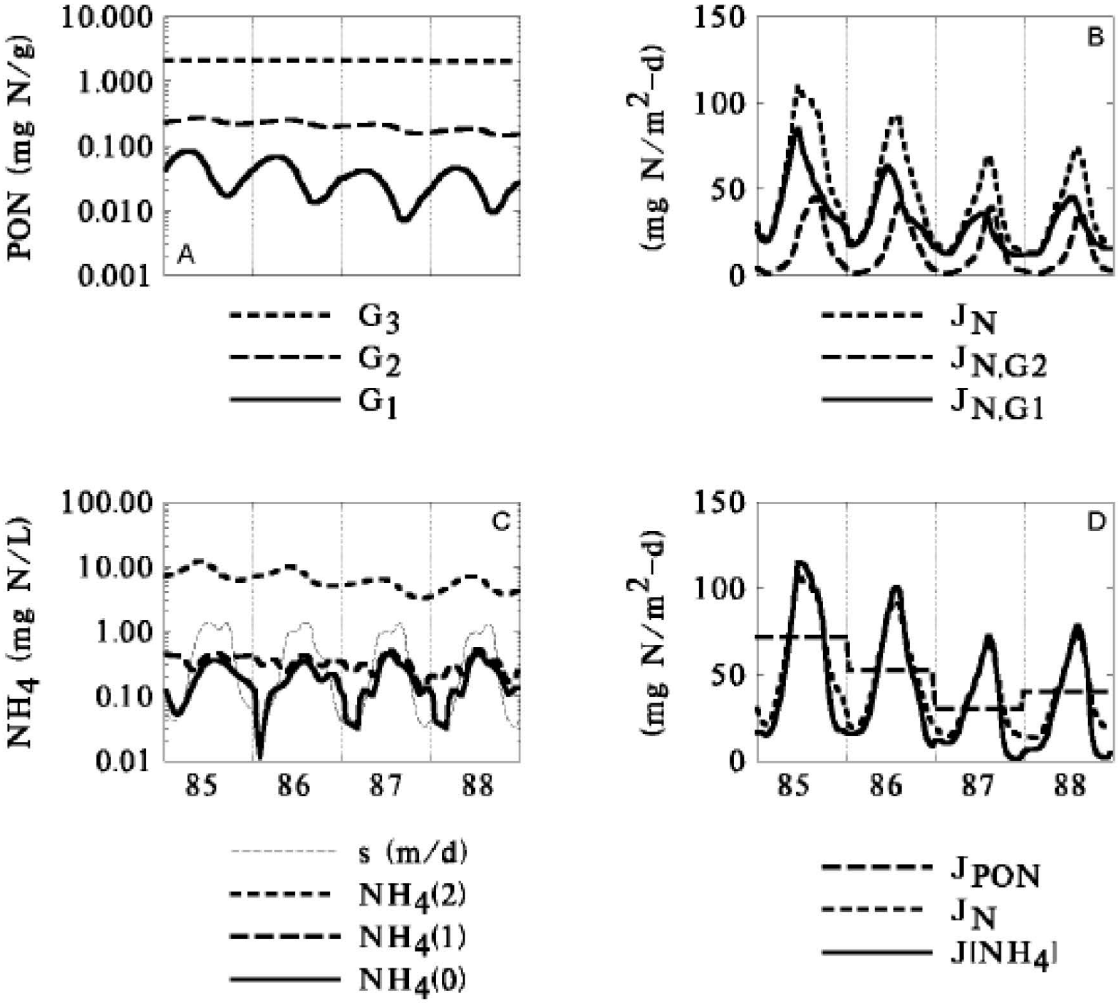
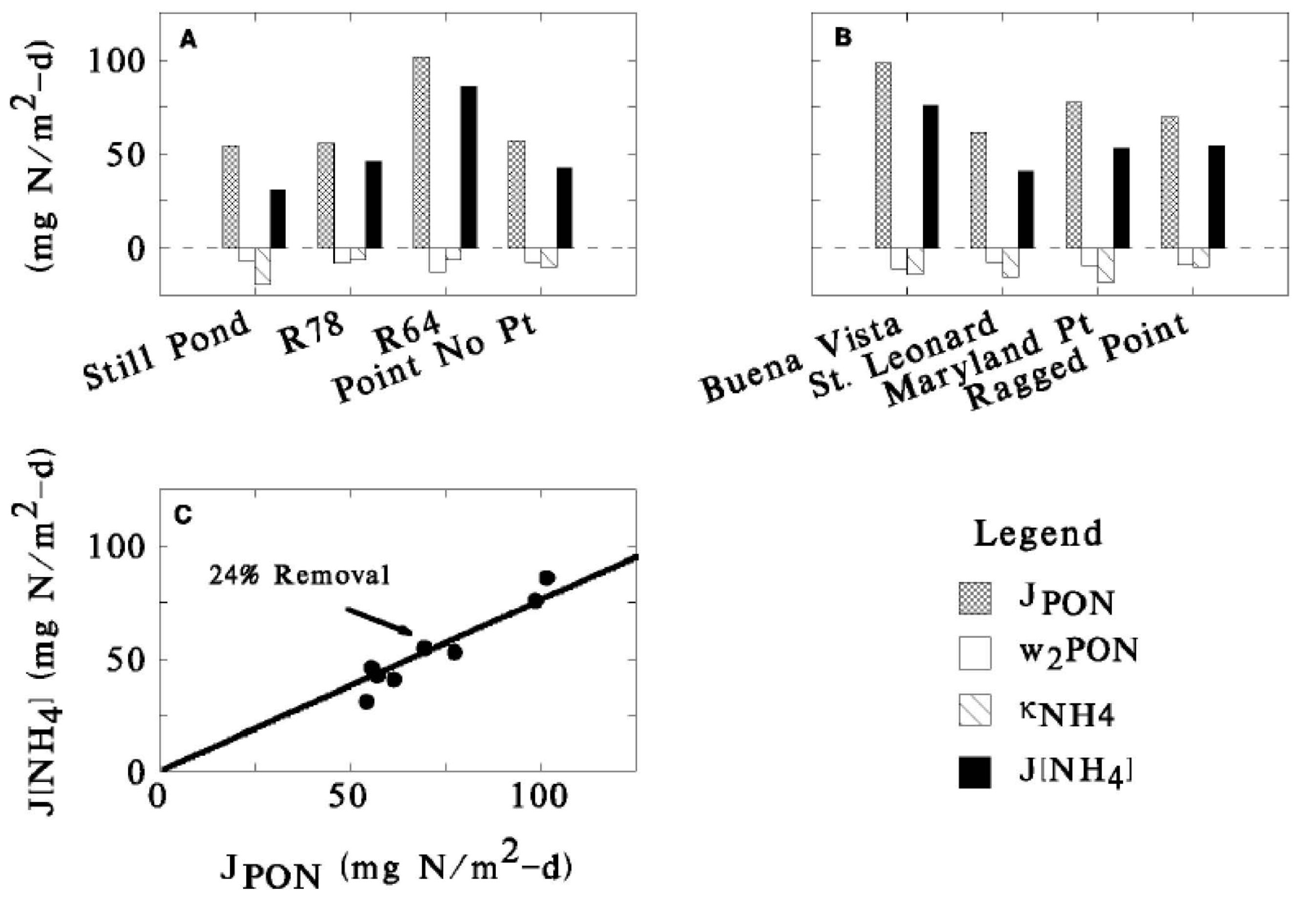


Table 12.6 Yearly Average Particulate Organic Nitrogen Depositional Fluxes J_{PON} (mg N/m^2-d)

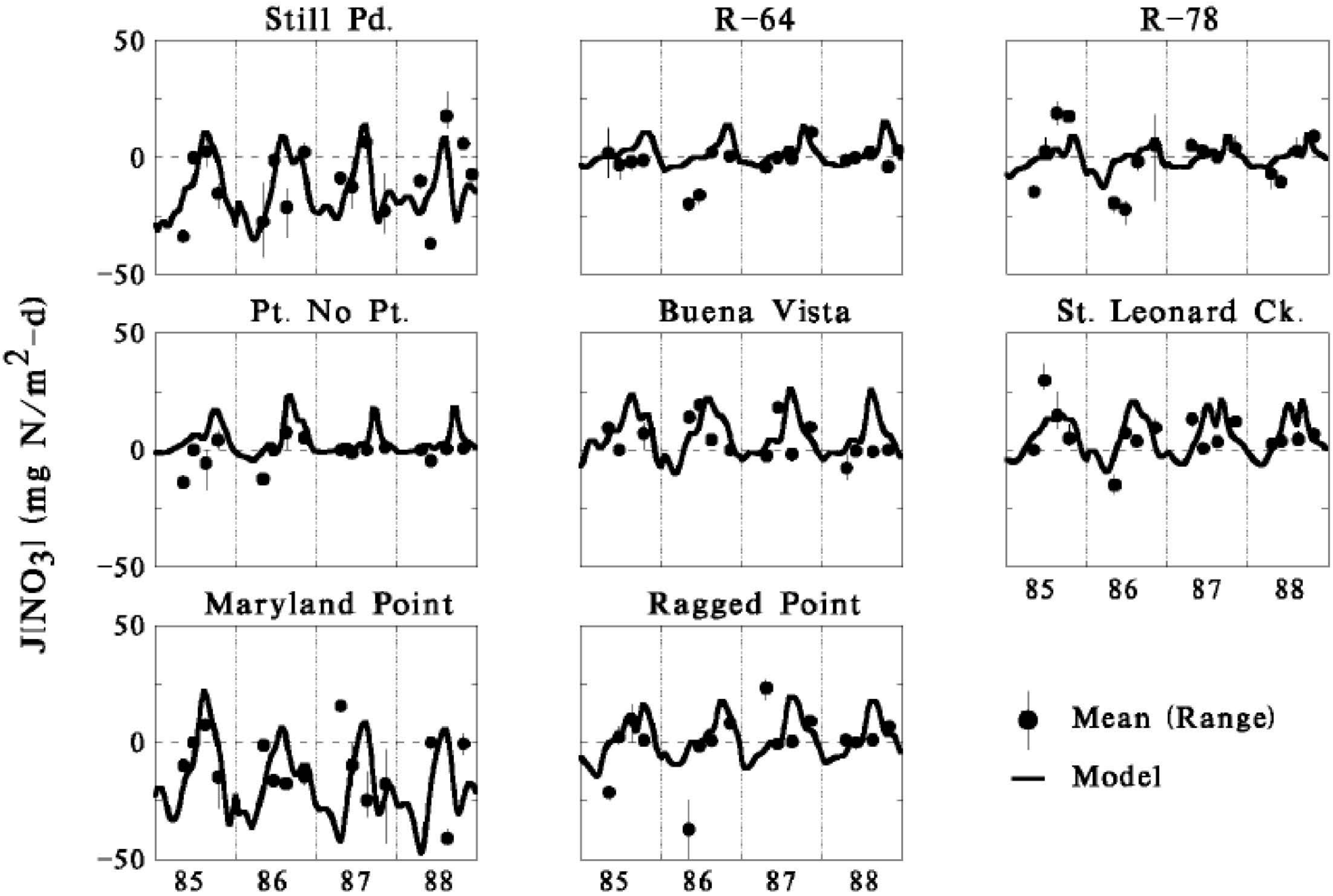
Station	1985	1986	1987	1988
Point No Point	66.6	61.3	34.1	50.0
R-64	114.2	110.0	50.0	110.0
R-78	71.7	52.2	30.0	40.0
Still Pond	57.0	80.0	47.4	30.0
St. Leo	64.0	47.1	72.3	57.9
Buena Vista	97.5	120.0	90.0	90.0
Ragged Point	75.0	125.0	40.0	30.0
Maryland Point	82.5	81.0	77.9	60.0

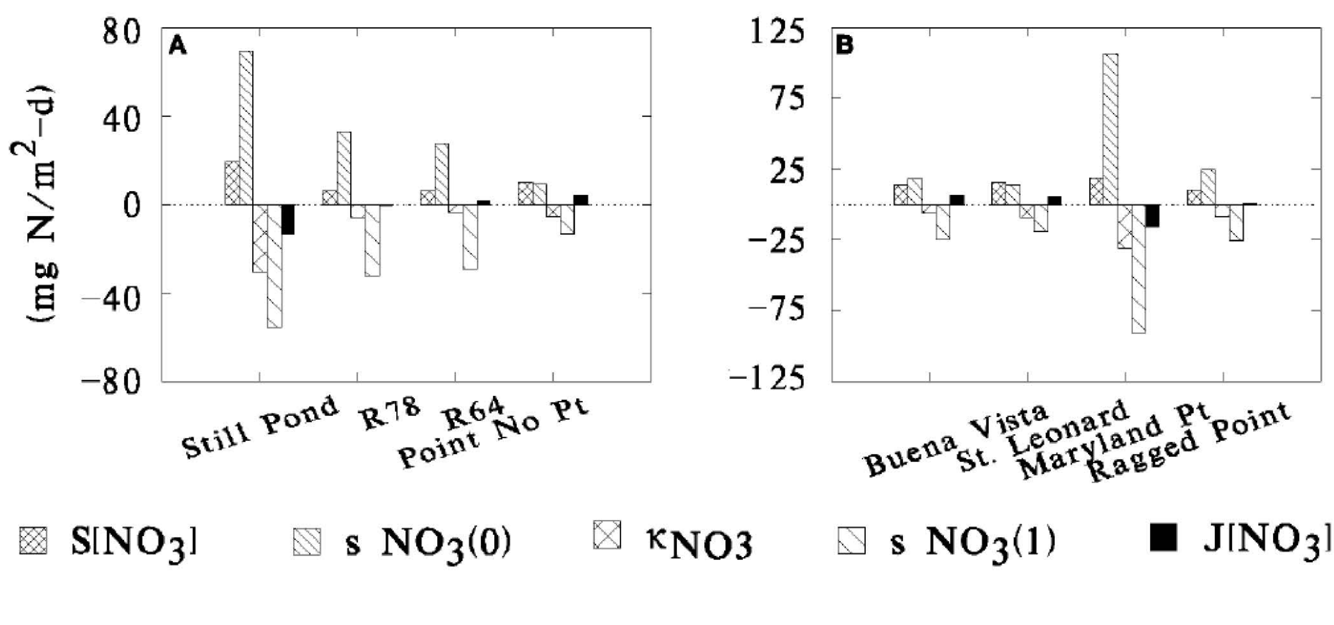
Ammonia Flux - Components



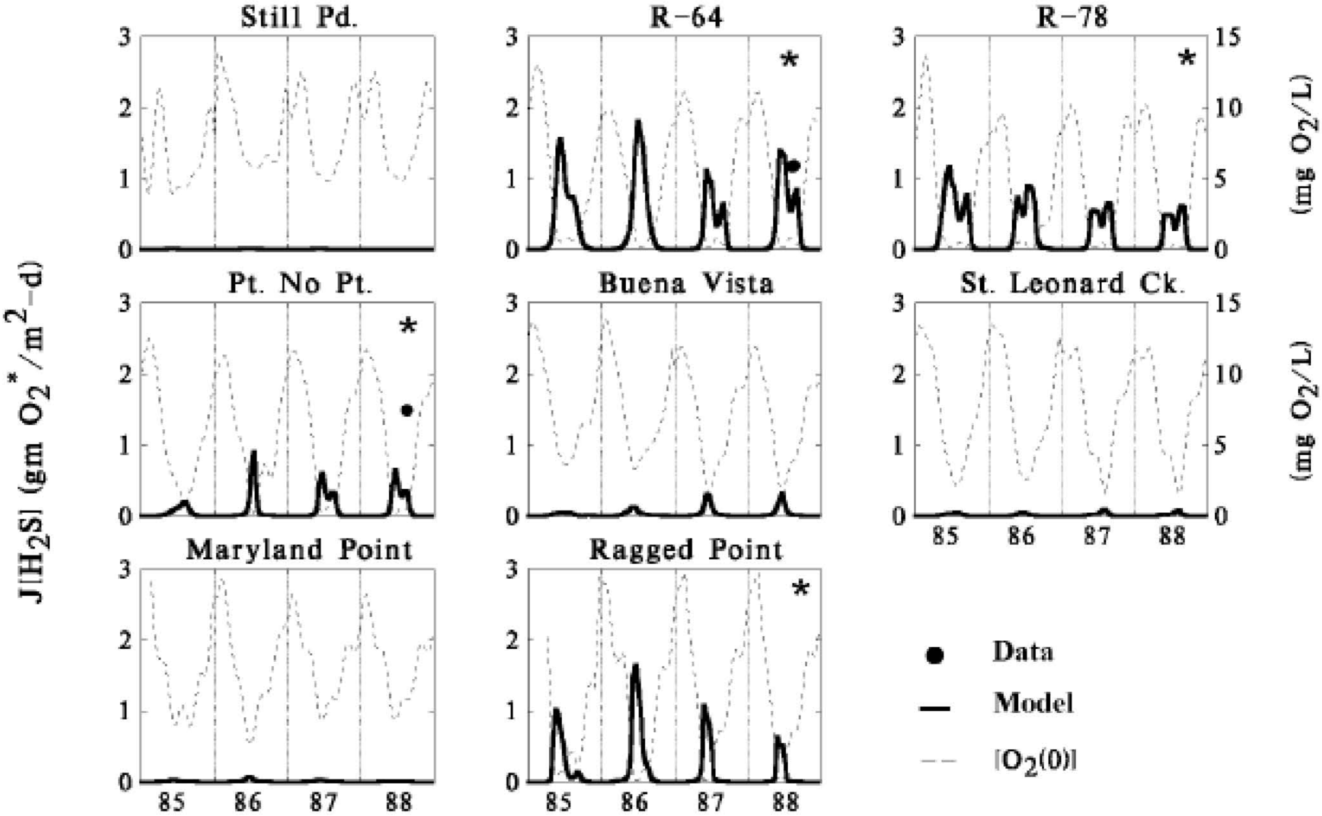


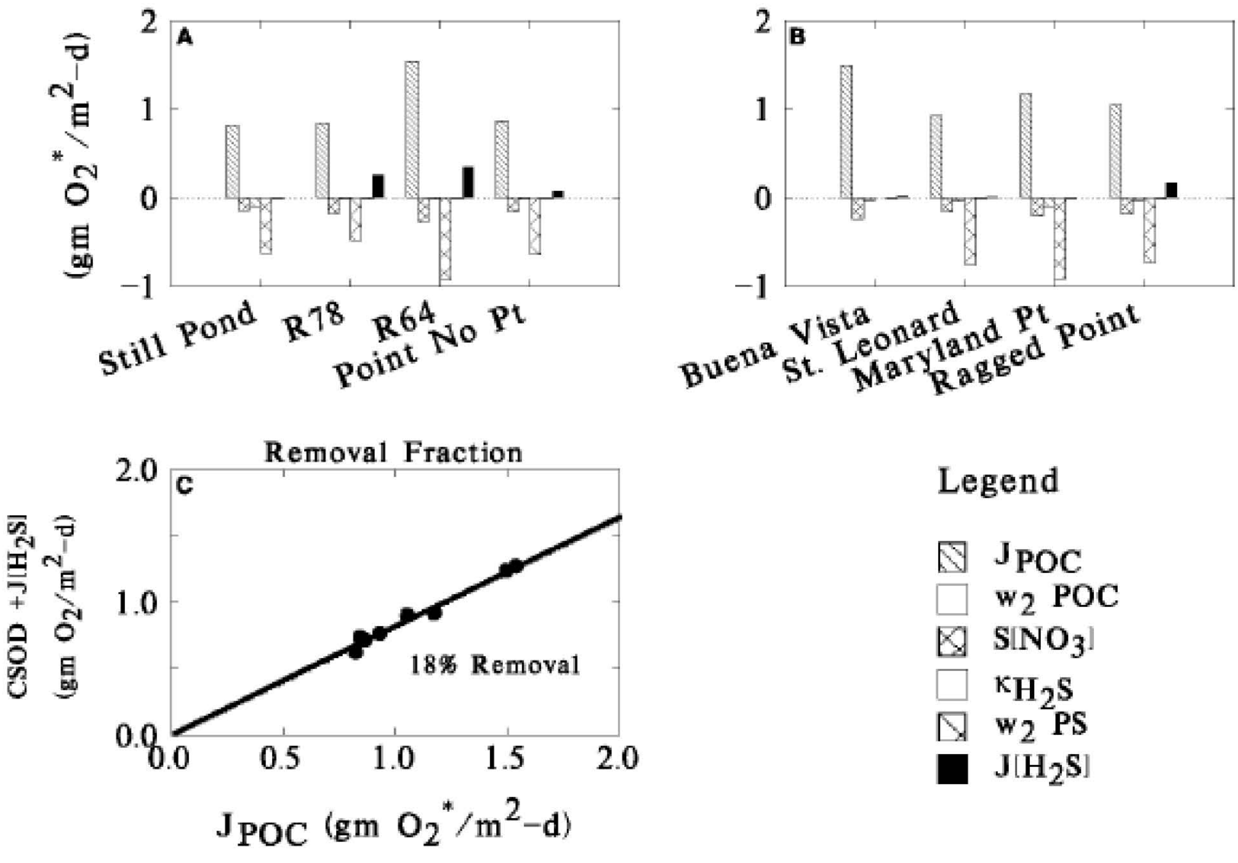
Nitrate Flux Model Calibration



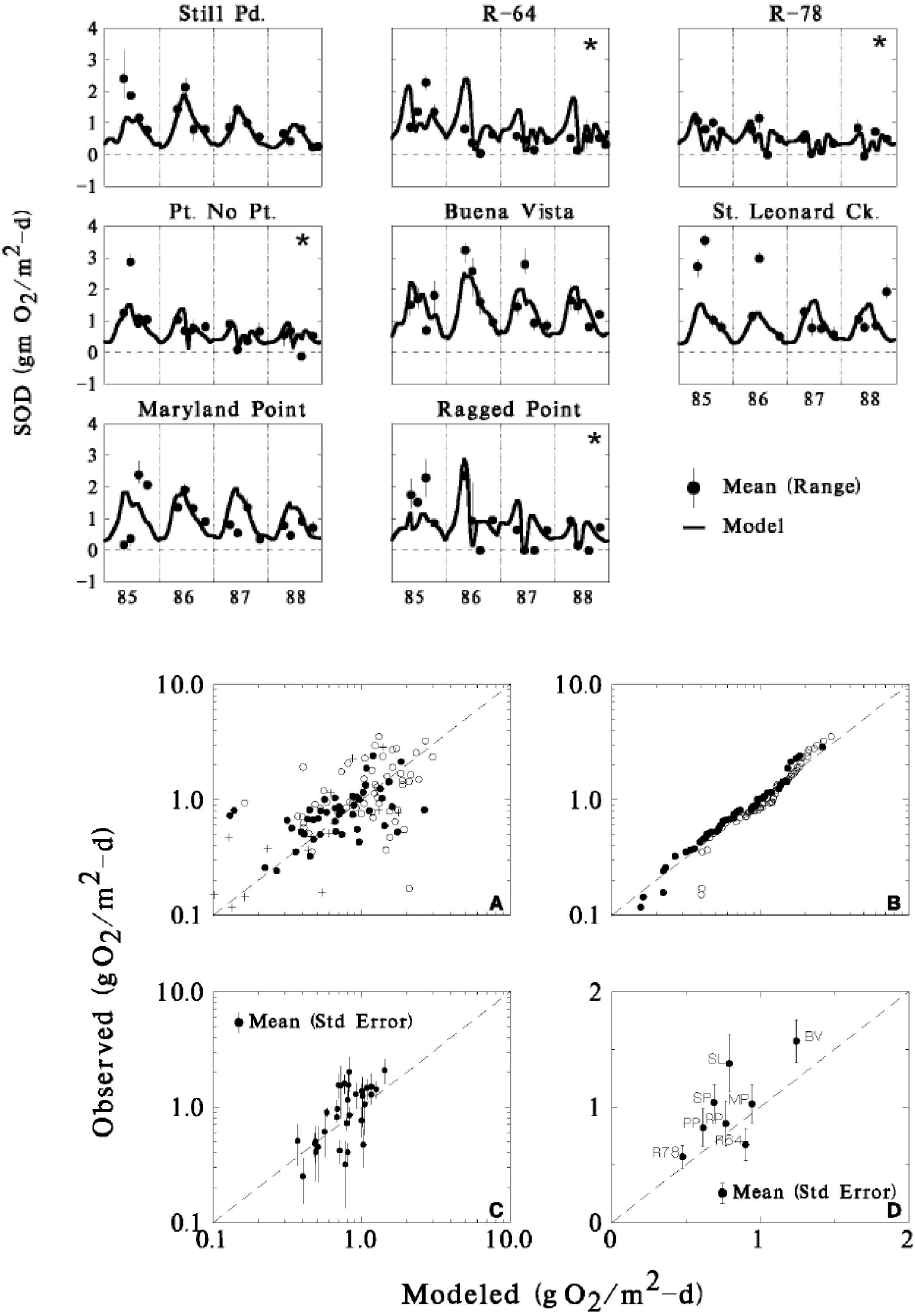


Hydrogen Sufide Flux Model



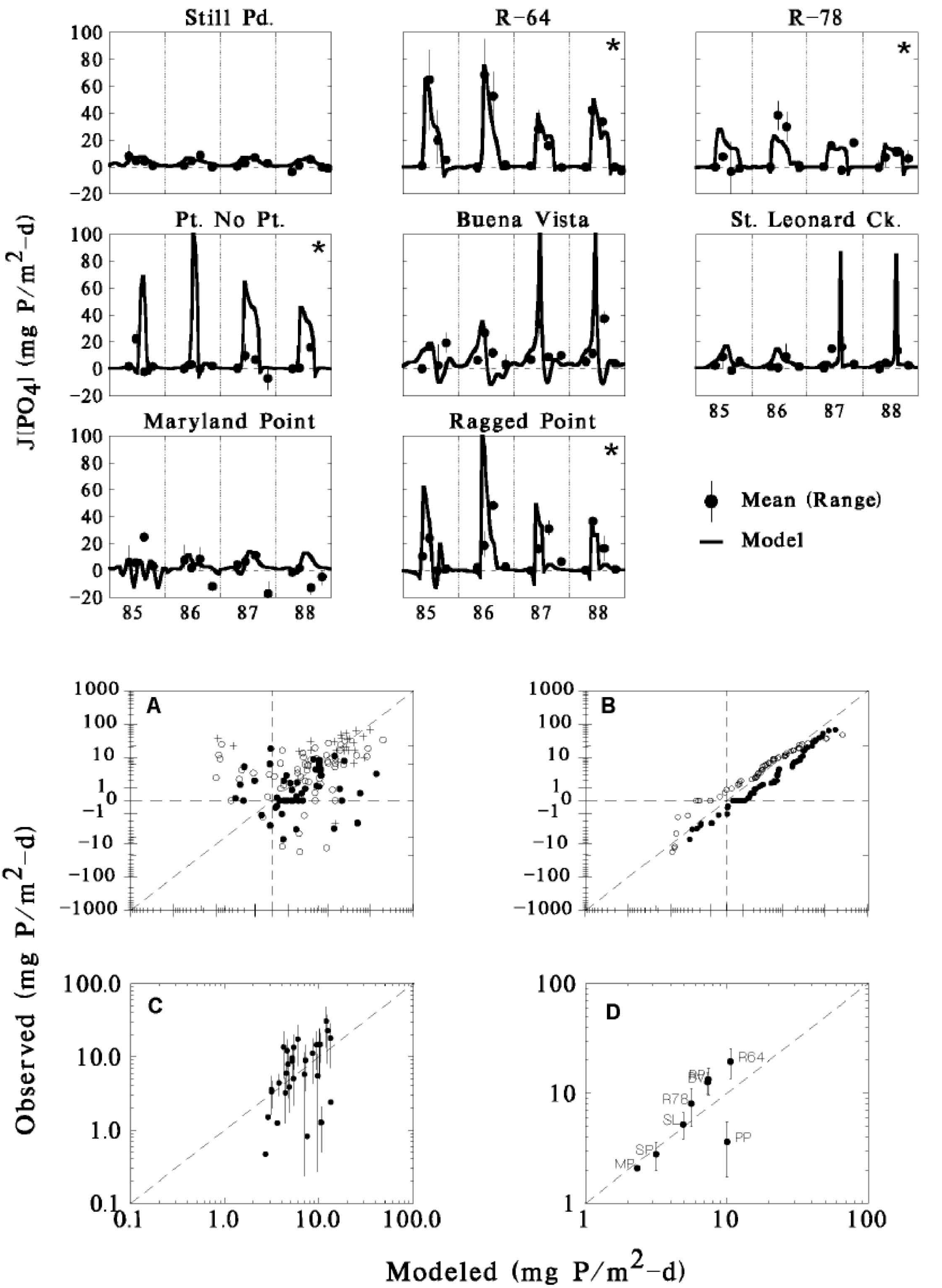


SOD Mocel

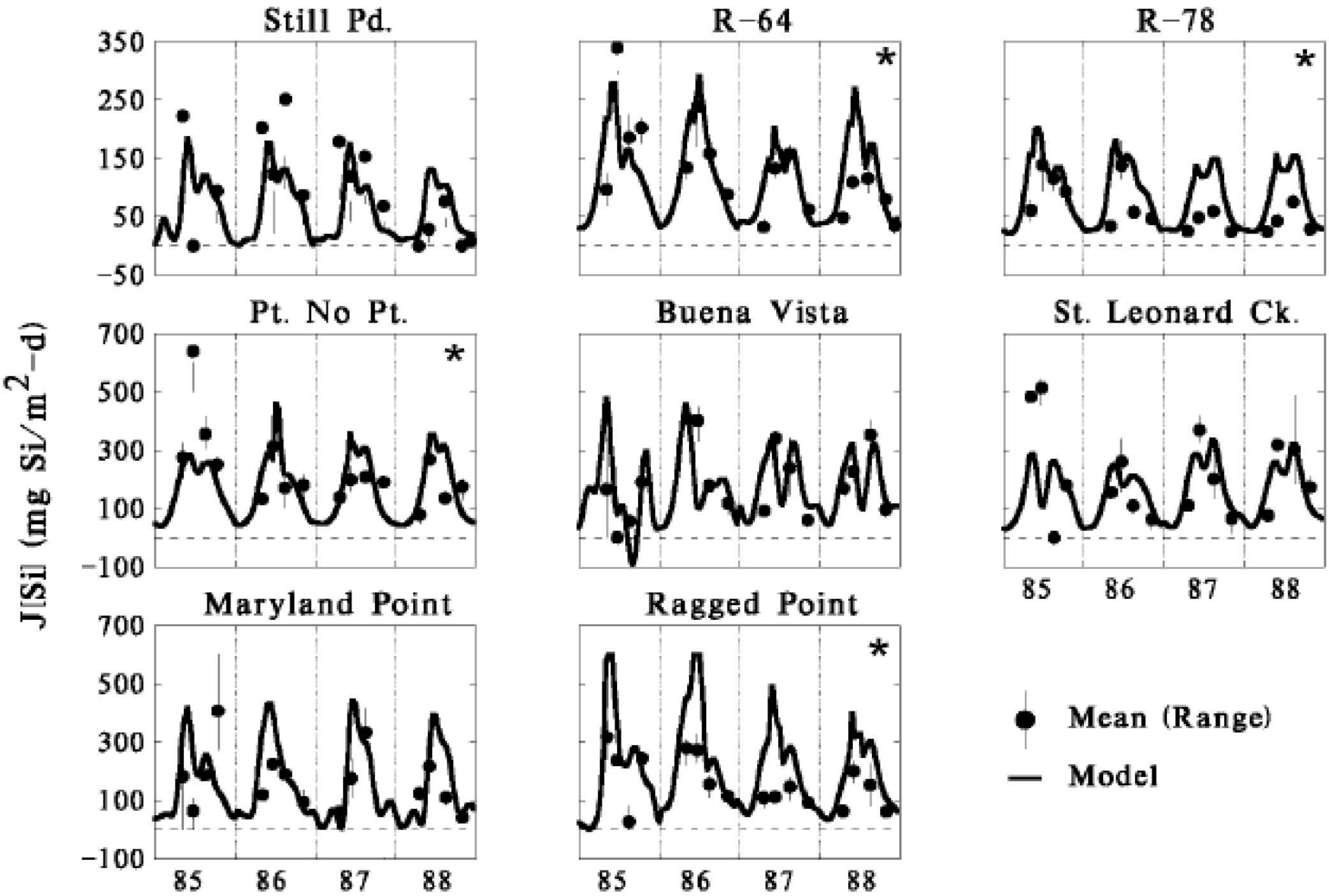


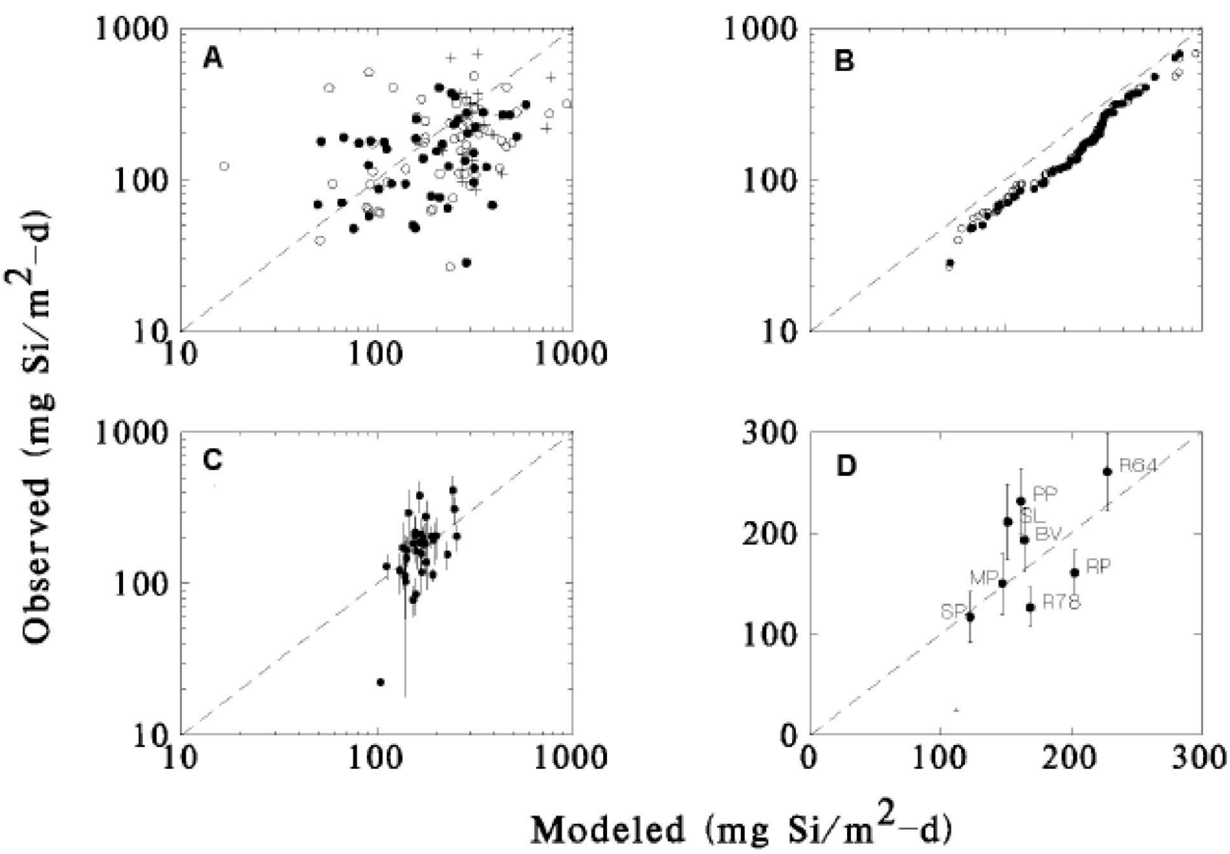
Still Pd.
R-64
R-78
Pt. No Pt.
Buena Vista
St. Leonard Ck.
Maryland Point
Ragged Point
SOD (gm O_2/m^2-d)
85
86
87
88
Mean (Range)
Model
Observed (g O_2/m^2-d)
Modeled (g O_2/m^2-d)
Mean (Std Error)
A
B
C
D
BV
SL
SP
MP
RP
PP
R64
R78

Phosphate Flux Model



Silica Flux Model





Di Toro, D.M., 2001. Sediment Flux Modeling.
Wiley-Interscience, New York ISBN: 0-471-13535-6

Contents

Nitrate Source from the Overlying Water

$$J[\mathrm{NO_3}] = -s\left(1 - \frac{s}{\kappa^2_{\mathrm{NO_3},1}/s + s + \kappa^*_{\mathrm{NO_3},2}}\right)[\mathrm{NO_3}(0)]$$

Normalized nitrate flux

$$\frac{J[\mathrm{NO_3}]}{[\mathrm{NO_3}(0)]} = -s\left(1 - \frac{s}{\kappa^2_{\mathrm{NO_3},1}/s + s + \kappa^*_{\mathrm{NO_3},2}}\right)$$

For large s

$$\frac{J[\mathrm{NO_3}]}{[\mathrm{NO_3}(0)]} = -\kappa^*_{\mathrm{NO_3},2} = -\left(\frac{1}{\kappa_{\mathrm{NO_3},2}} + \frac{1}{K_{\mathrm{L12}}}\right)^{-1}$$

Constant, limited by either mass transfer K_{L12} or denitrification rate $\kappa_{\mathrm{NO_3},2}$

Nitrate Source from the Overlying Water

For small s

$$\frac{J[\mathrm{NO_3}]}{[\mathrm{NO_3(0)}]} = -s \qquad\qquad s \longrightarrow 0$$

$$\frac{J[\mathrm{NO_3}]}{[\mathrm{NO_3(0)}]} = -s = -\frac{\mathrm{SOD}}{[\mathrm{O_2(0)}]} = \frac{J[\mathrm{O_2}]}{[\mathrm{O_2(0)}]}$$

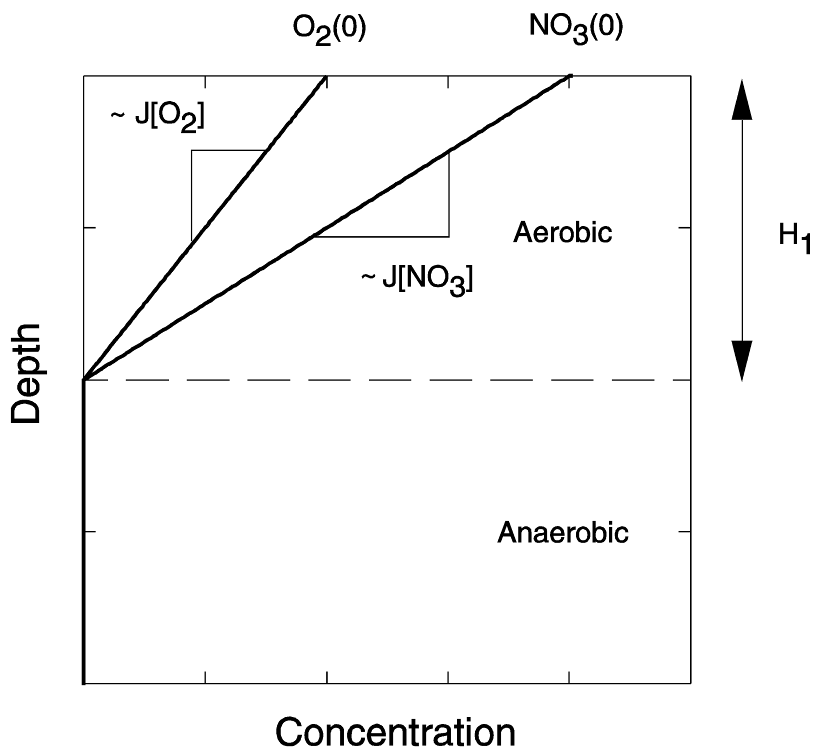


Figure 2: Vertical profiles of oxygen and nitrate.