QUAL2K

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

QUAL2K WORKSHOP: INTRODUCTION*

Steve Chapra
Tufts University

- ***Rationale and Overview***
- ***Segmentation and Hydraulics***

* Abbreviated for Region 6 Modeling Workshop, November 2013, by Robert Ambrose

QUAL2K

- *Steady-state, 1-D Mainstem River*
- *Fast C (BOD), Slow C (BOD), organic N, NH3, NO3, organic P, SRP, oxygen, phytoplankton, FIXED PLANTS, suspended solids, conservative/color*
- *Heat budget*
- *Point and distributed loads and abstractions*

QUAL2K

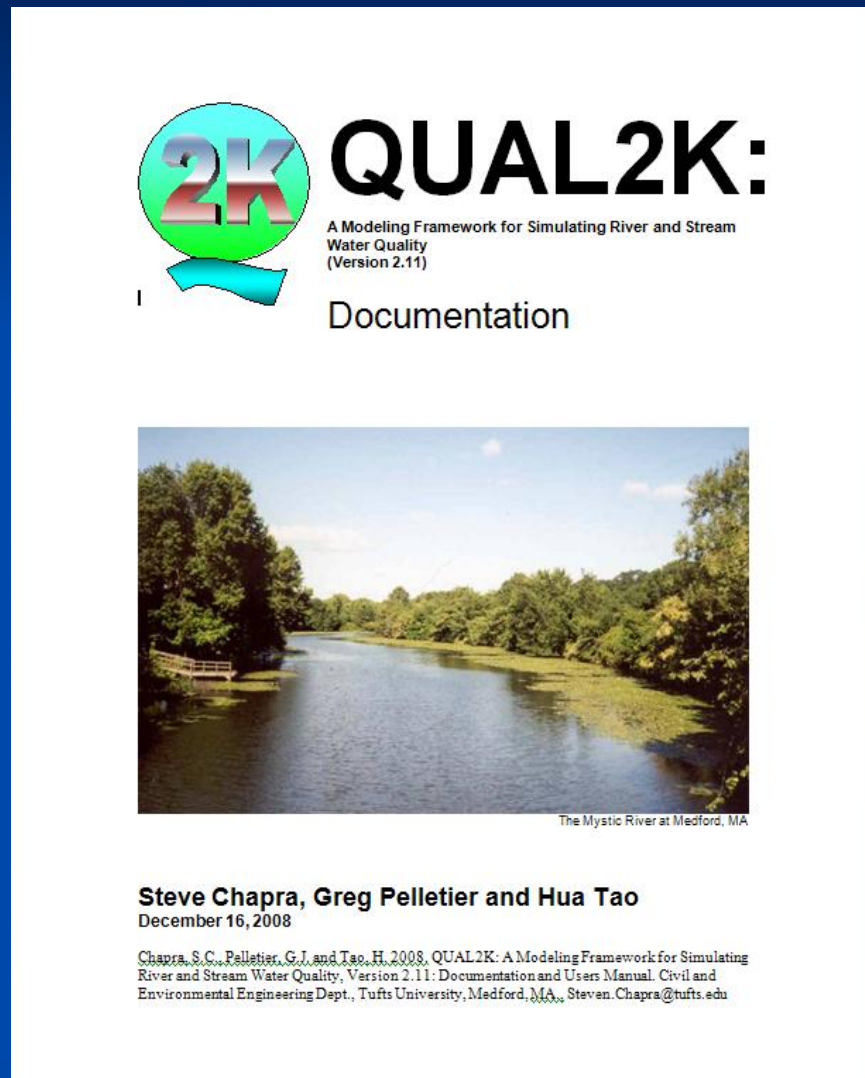
- Speciates carbon
- Anoxia
  - Shuts down oxidation at low DO
  - Denitrification
- Fixed plants
- SOD and sediment nutrient fluxes calculated

QUAL2K

- Software environment and interface
- Model segmentation
- Carbon speciation
- Anoxia and denitrification
- Sediment-water interactions
- Bottom plants
- Light extinction
- pH
- Pathogens

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

QUAL2K Documentation



QUAL2K:

A Modeling Framework for Simulating River and Stream Water Quality
(Version 2.11)

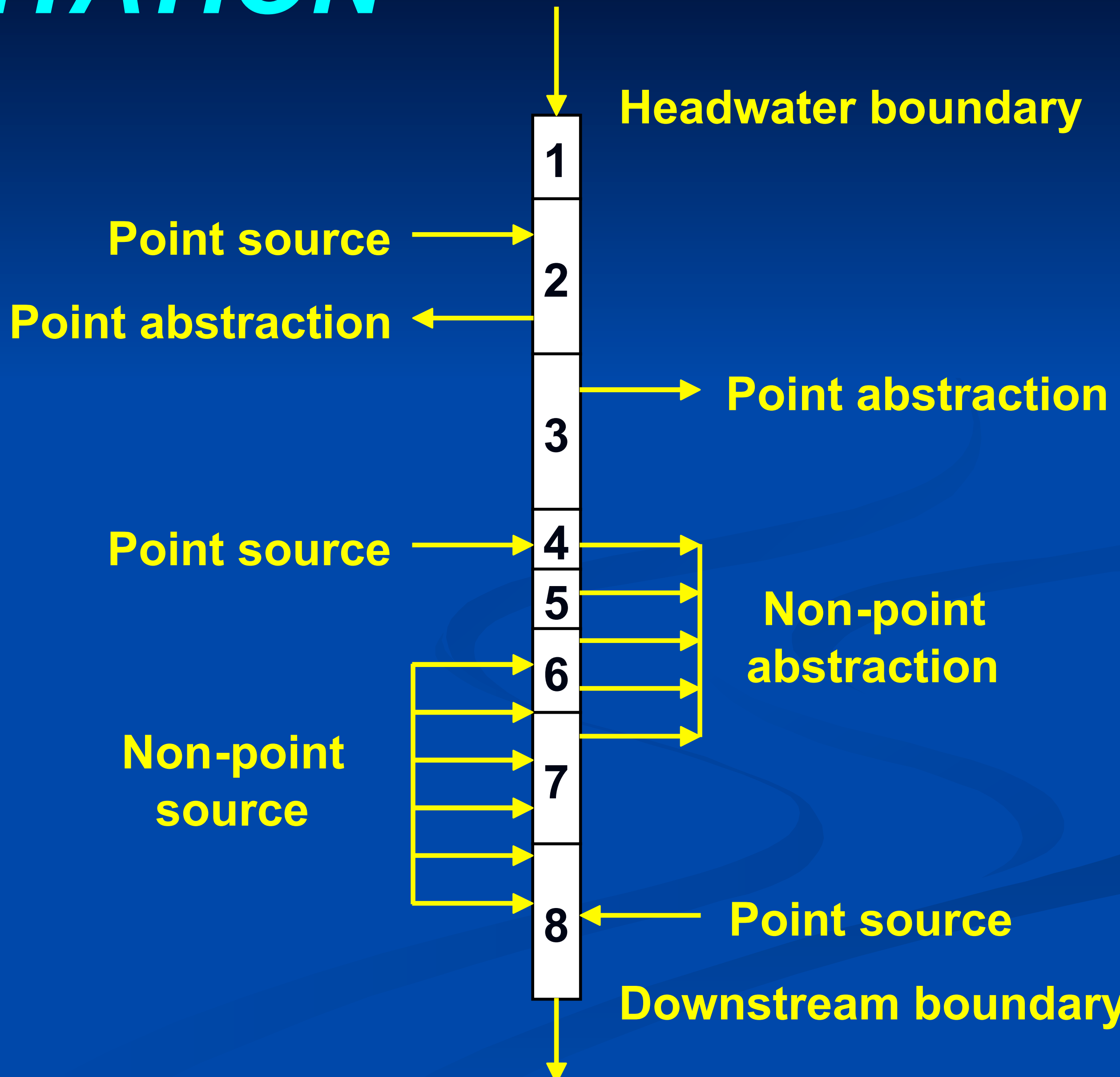
Documentation

The Mystic River at Medford, MA

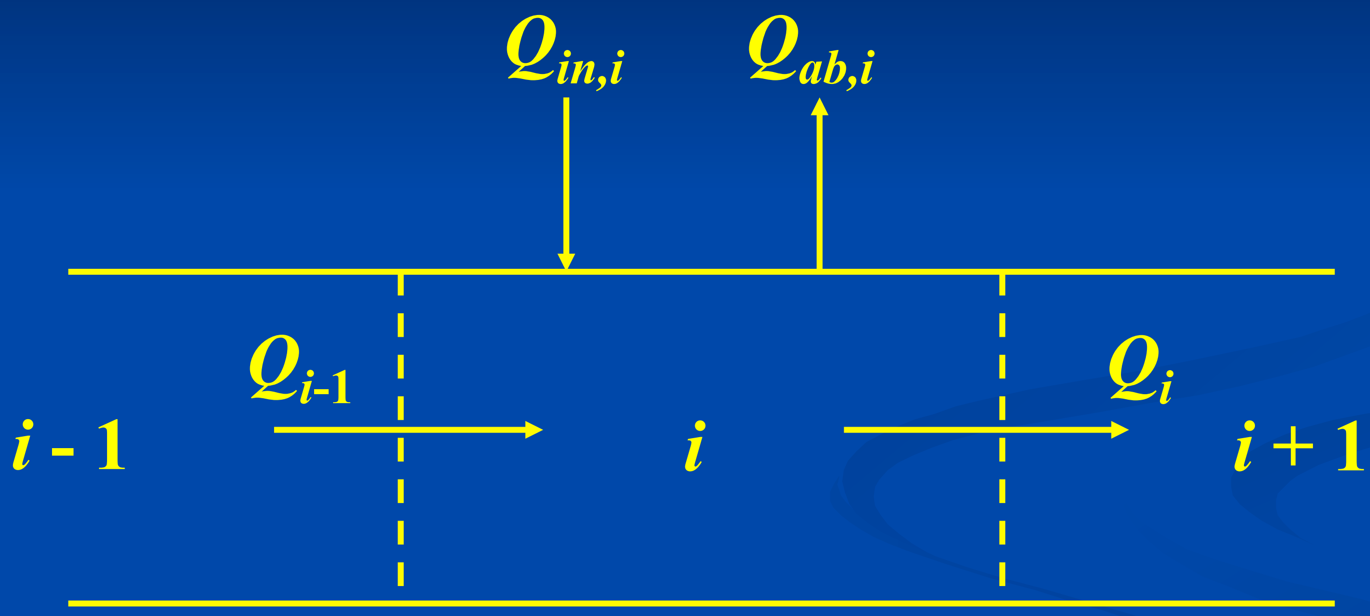
Steve Chapra, Greg Pelletier and Hua Tao
December 16, 2008

Chapra, S.C., Pelletier, G.J. and Tao, H. 2008. QUAL2K: A Modeling Framework for Simulating River and Stream Water Quality, Version 2.11: Documentation and Users Manual. Civil and Environmental Engineering Dept., Tufts University, Medford, MA., Steven.Chapra@tufts.edu

SEGMENTATION

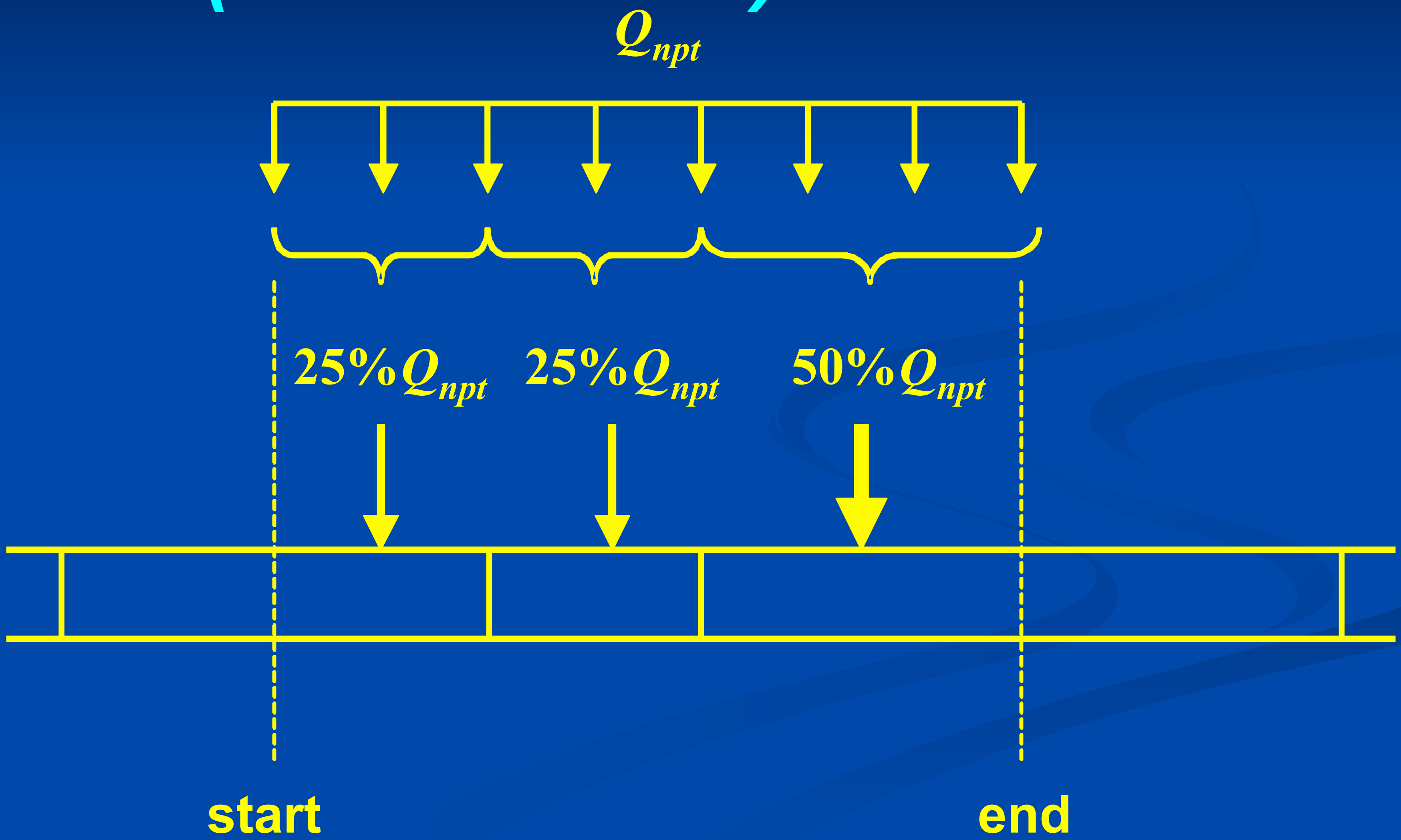


FLOW BALANCE

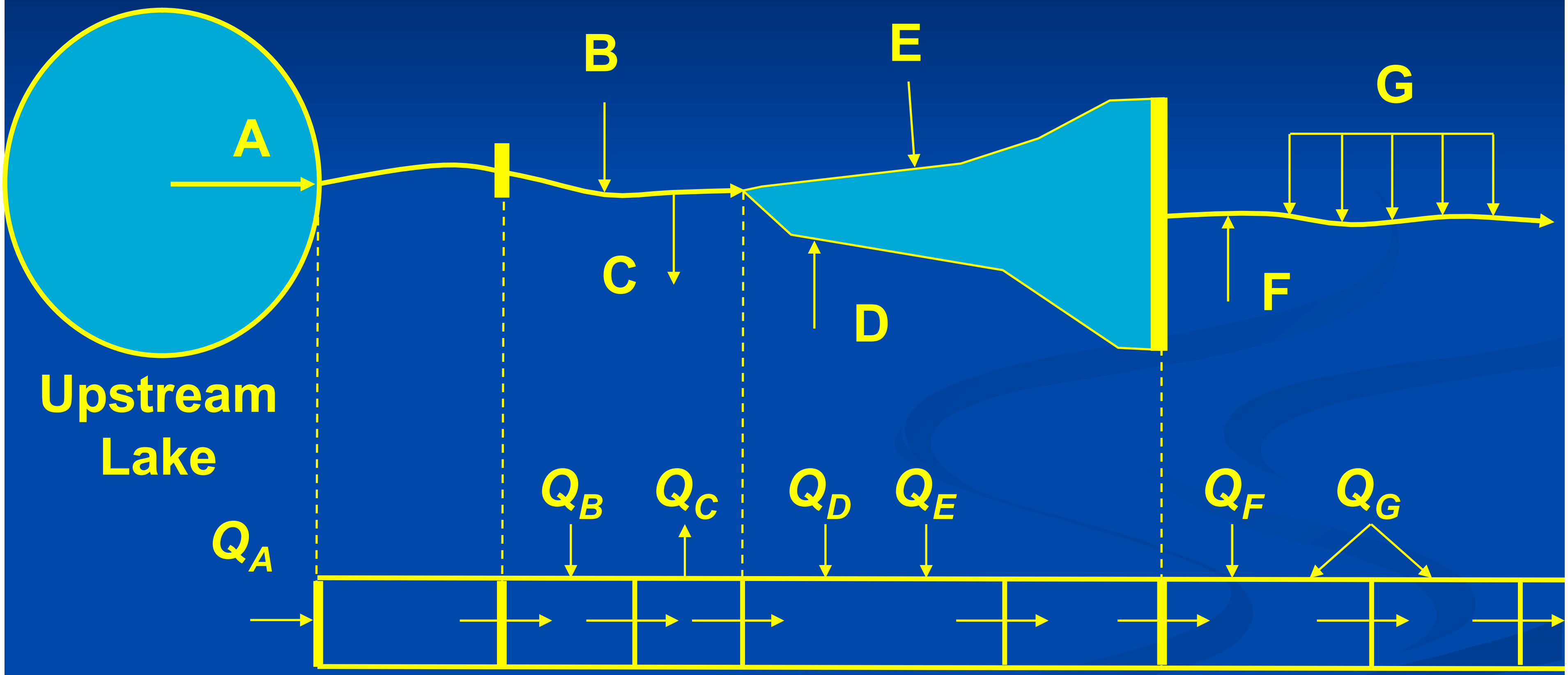


$$Q_i = Q_{i\text{-}1} + Q_{in,i} - Q_{ab,i}$$

DISTRIBUTED (NON-POINT) LOADS

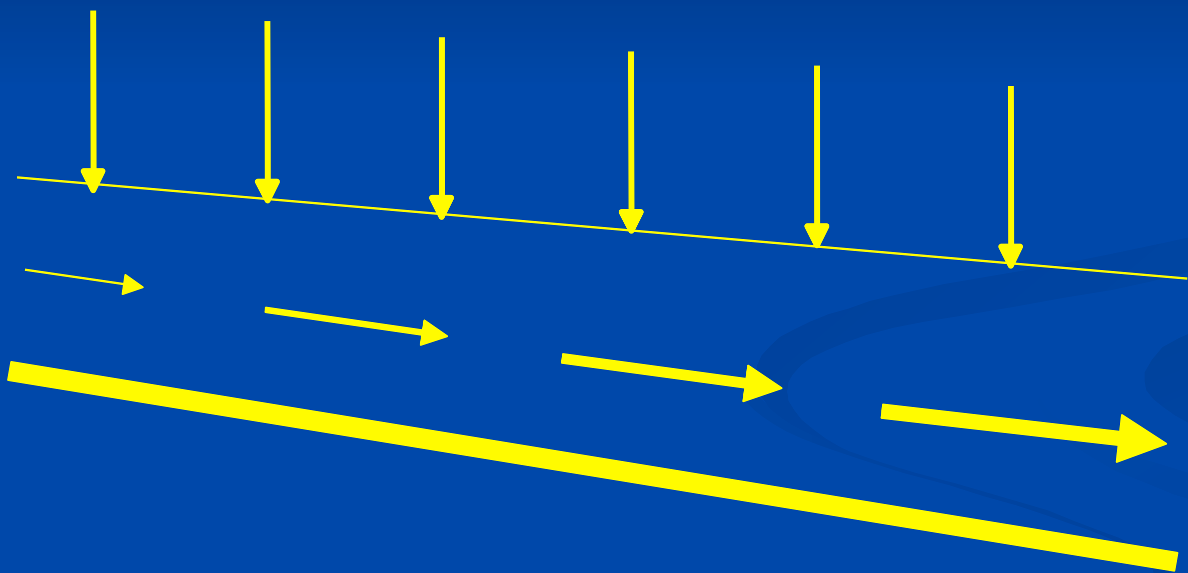


STEADY-STATE FLOW BALANCE



WHAT HAPPENS WHEN YOU ADD FLOW TO A SLOPING CHANNEL?

The water velocity and depth increase



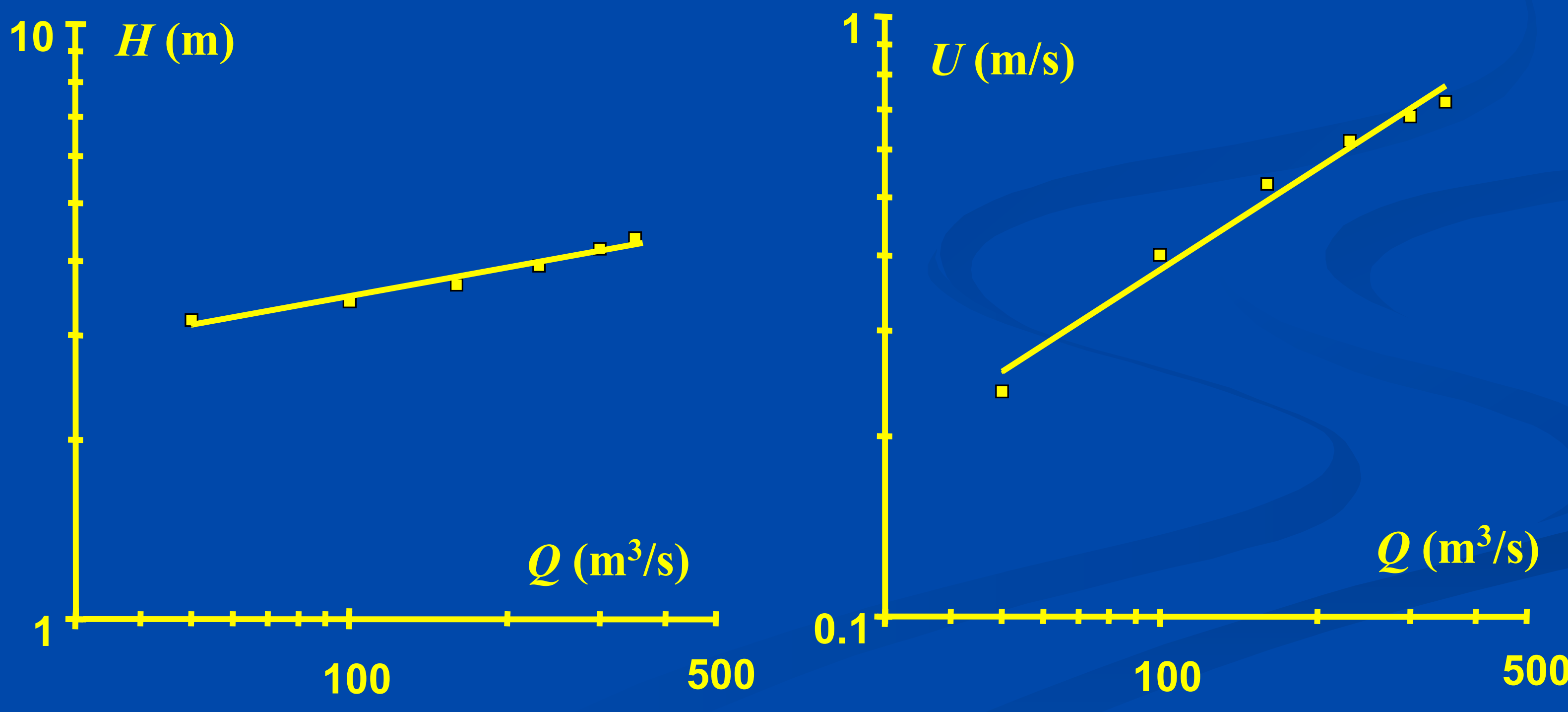
Given $Q_{outflow}$, compute depth (H) and velocity (U):

- **Continuity and Manning equation**
- **Rating Curves**

RATING CURVES

$$H = 1.6487\, Q^{0.1622}$$

$$U = 0.0279\, Q^{0.5652}$$



RIVER HYDROGEOMETRY (STEADY)

Q

Manning → Rating Curves

U, H

$$A_c = Q/U$$

$$B = A_c / H$$

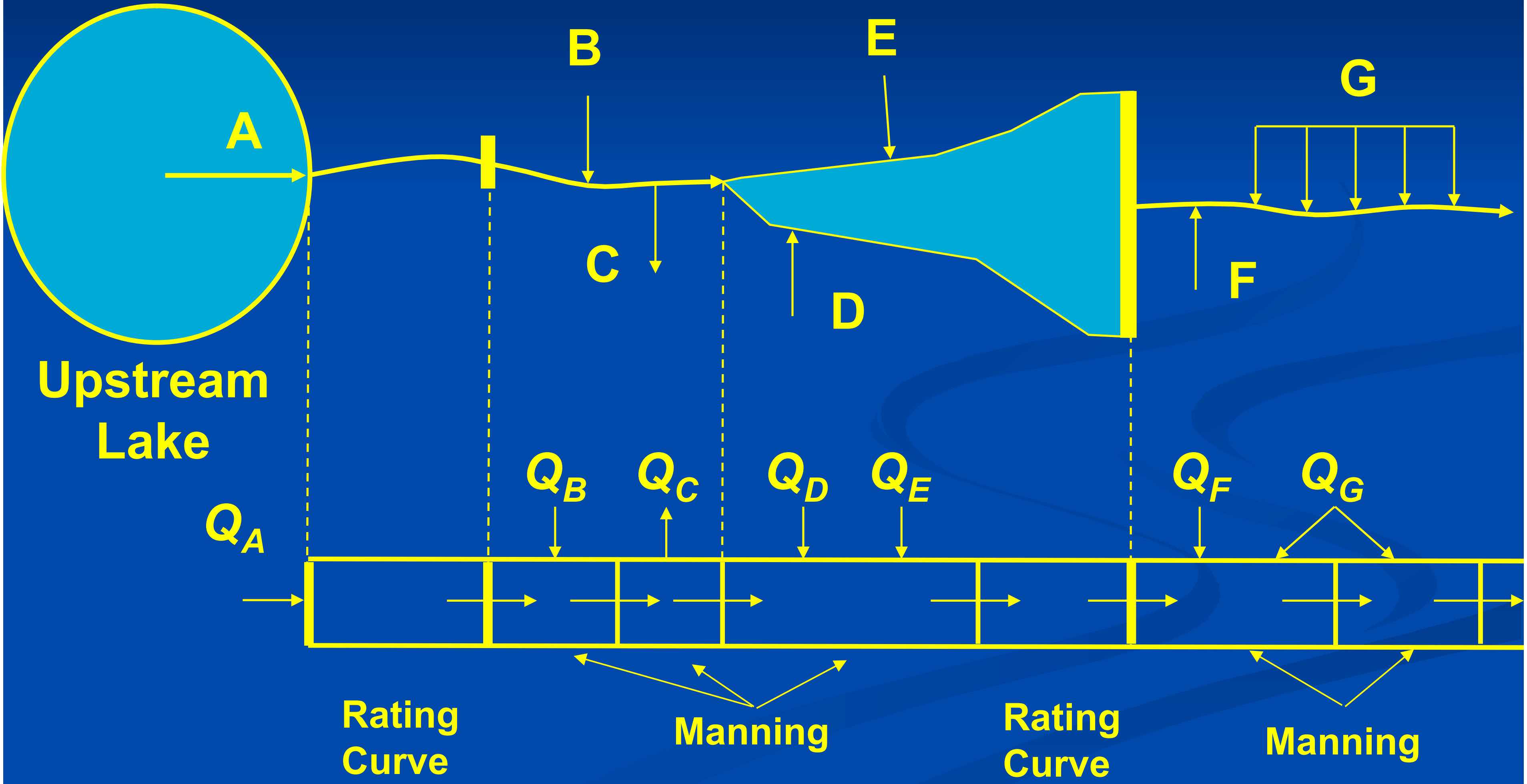
$$A_s = \Delta x \, B$$

$$V = B \, H \, \Delta x$$

$$\tau_w = \Delta x / U = V/Q$$

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

STEADY-STATE FLOW BALANCE



LONGITUDINAL DISPERSION

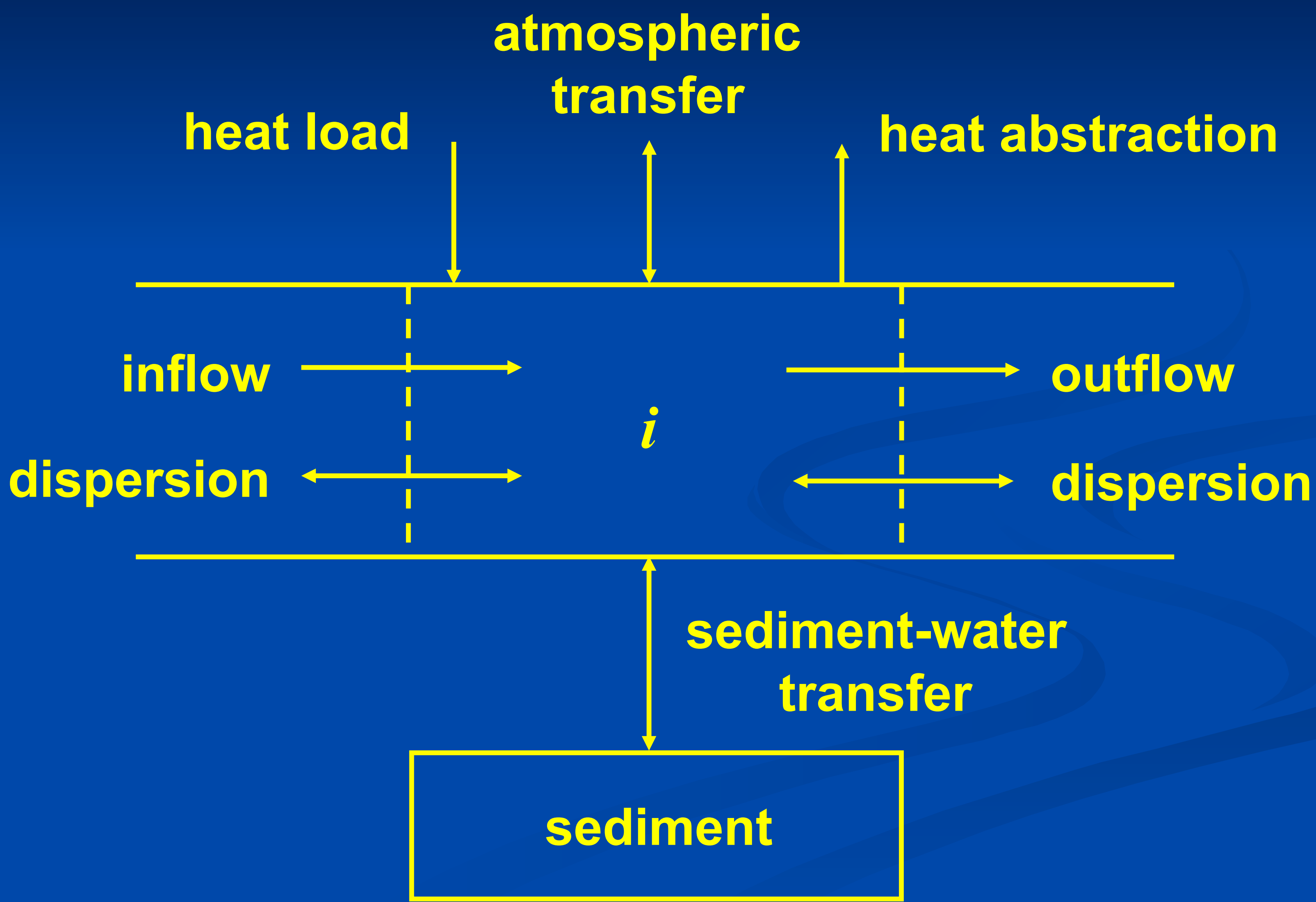
$$E = 0.011 \frac{U^2 B^2}{H U^*}$$

$$U^* = \sqrt{gHS}$$

QUAL2K WORKSHOP:
TEMPERATURE MODELING

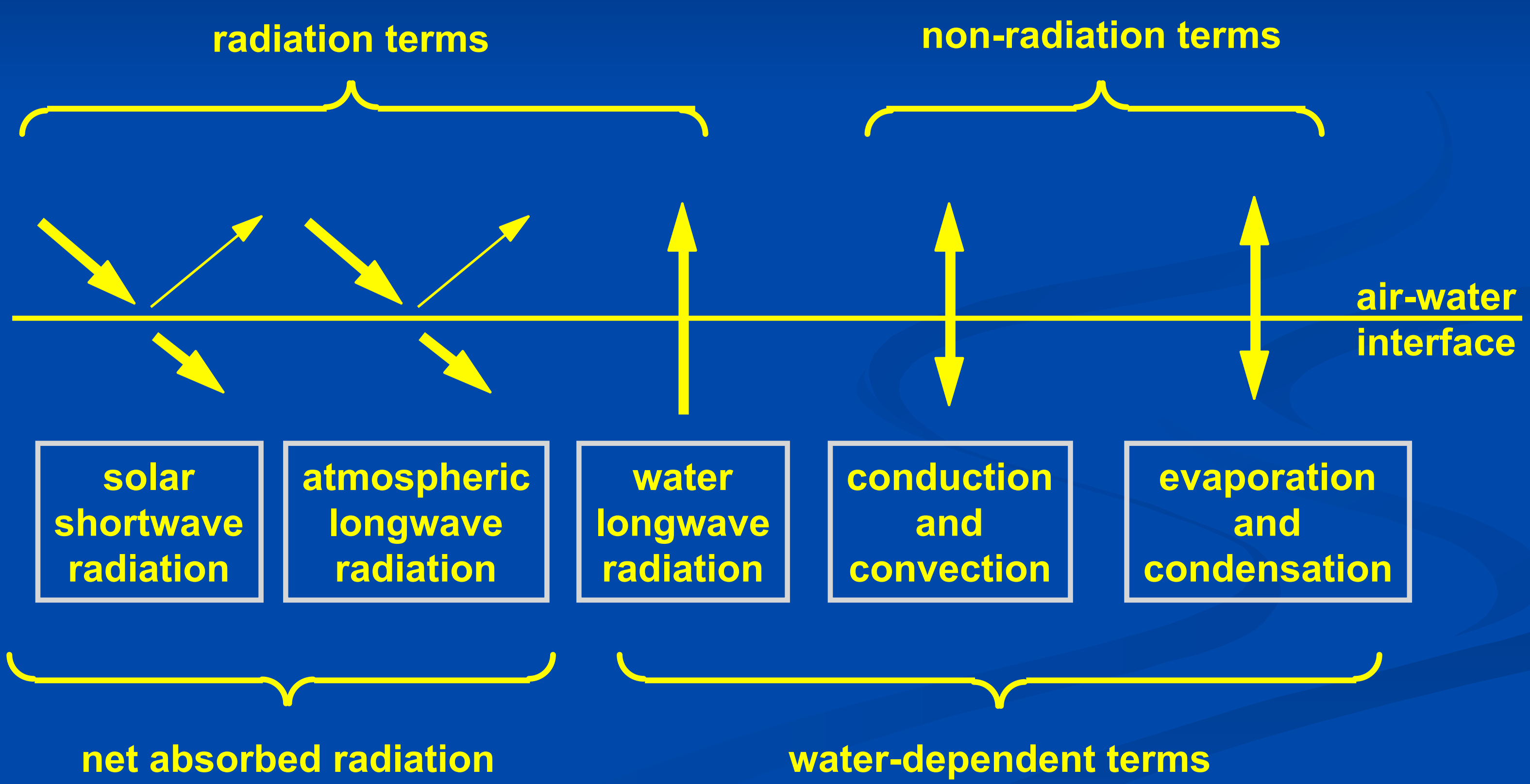
- Heat Balance
- Surface Heat Flux
- Meteorological Data
- Air-Water Converter
- Sediment Heat Flux

Q2K


atmospheric
transfer
heat load
heat abstraction
inflow
outflow
i
dispersion
dispersion
sediment-water
transfer
sediment

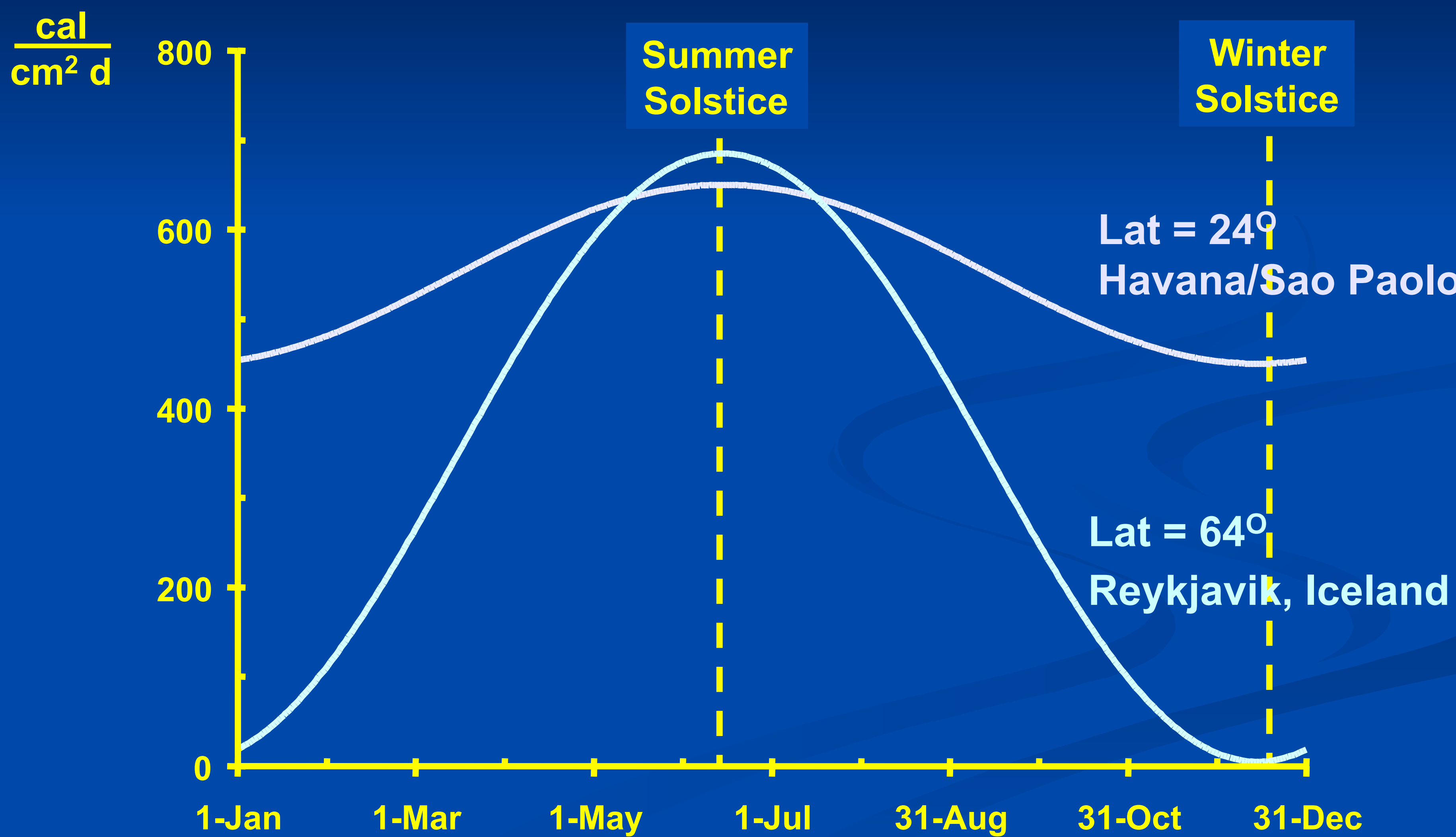
Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

SURFACE HEAT BALANCE



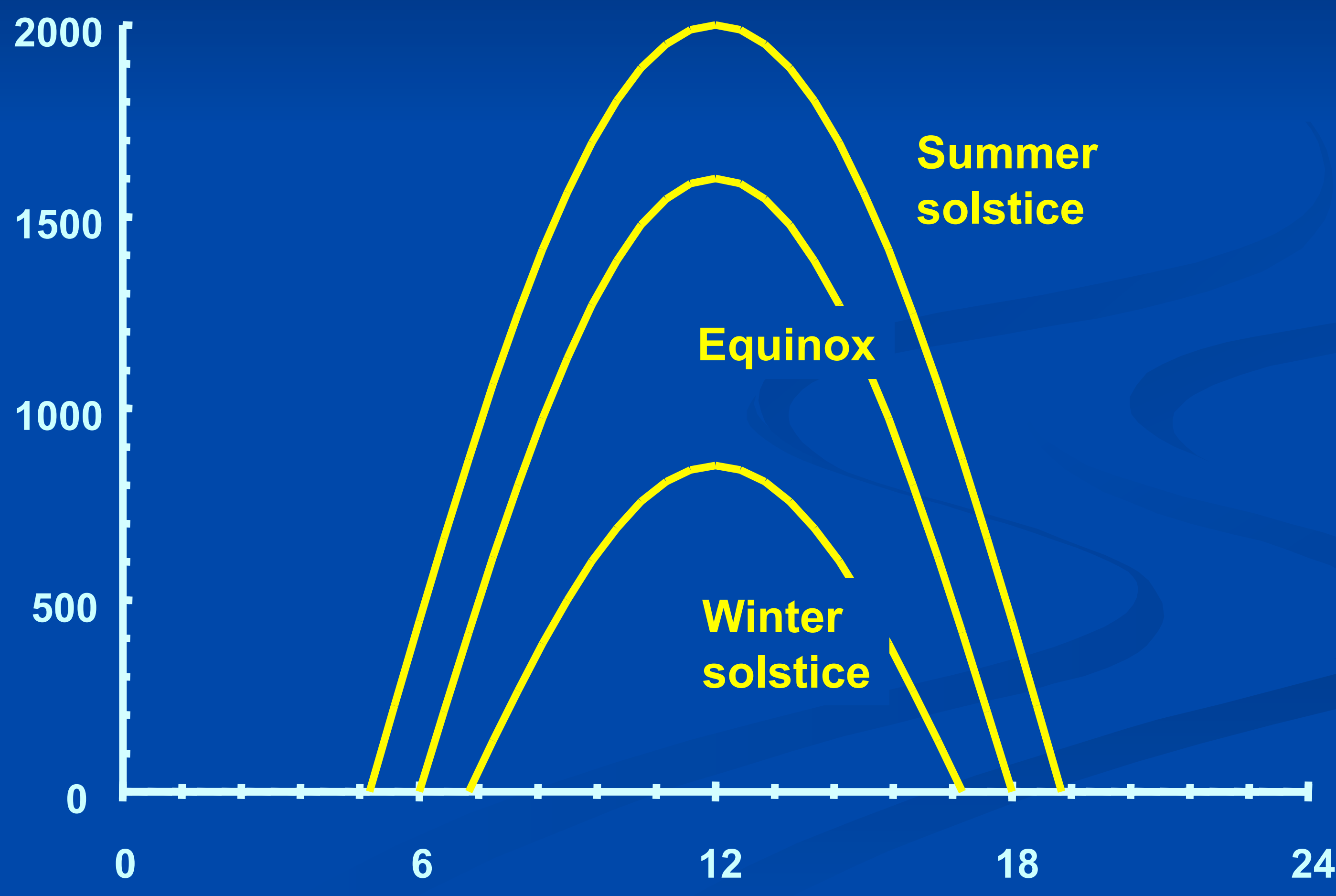
Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

ANNUAL SOLAR RADIATION



Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

DAILY SOLAR RADIATION



WHAT YOU NEED??? (METEOROLOGICAL DATA)

Air Temperature

Dew Point Temperature

$$J = J_{sn} + \sigma (T_{\text{air}} + 273.15)^4 \left(A + 0.031 \sqrt{e_{air}} \right) (1 - R_L)$$

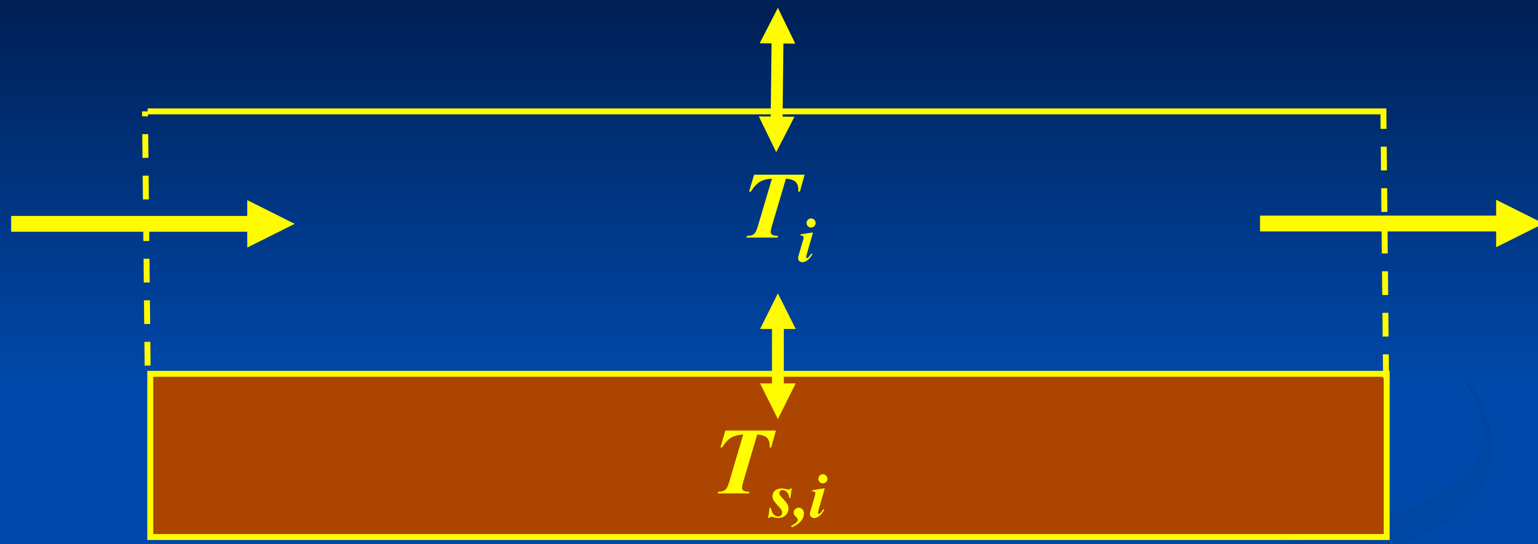
$$- \varepsilon \sigma (T_s + 273.15)^4 - c_1 f(U_w)(T_s - T_{\text{air}}) - f(U_w)(e_s - e_{\text{air}})$$

Solar (Cloud Cover)

Wind Speed

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

SEDIMENT HEAT BUDGET



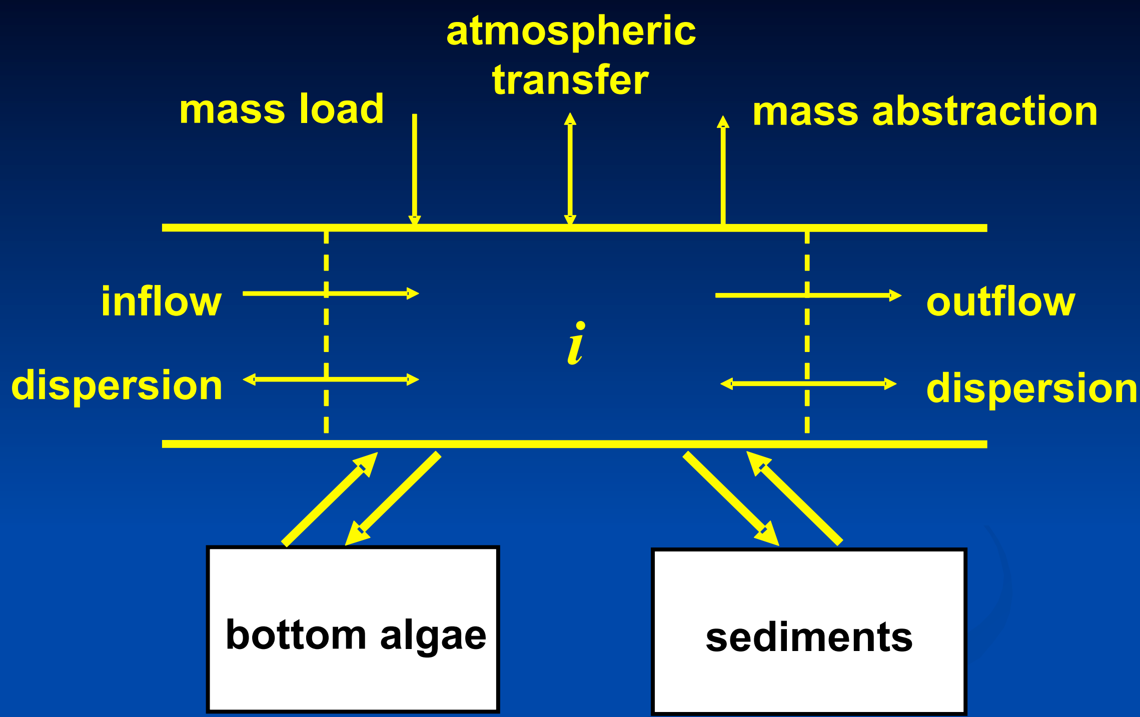
$$\frac{dT_{s,i}}{dt} = \frac{J_{s,i}}{\rho C_p H_{si}}$$

$$J_{s,i} = \frac{\alpha_s}{H_s}\left(T_i - T_{si}\right)$$

Q2K WATER QUALITY

Variable	Symbol	Units*
Conductivity	s	µmhos
Inorganic suspended solids	m_i	mgD/L
Dissolved oxygen	o	mgO_2/L
Slowly reacting CBOD	c_s	mgO_2/L
Fast reacting CBOD	c_f	mgO_2/L
Organic nitrogen	n_o	µgN/L
Ammonia nitrogen	n_a	µgN/L
Nitrate nitrogen	n_n	µgN/L
Organic phosphorus	p_o	µgP/L
Inorganic phosphorus	p_i	µgP/L
Phytoplankton	a_p	µgA/L
Phytoplankton nitrogen	IN_p	µgN/L
Phytoplankton phosphorus	IP_p	µgP/L
Detritus	m_o	mgD/L
Pathogen	X	cfu/100 mL
Alkalinity	Alk	$mgCaCO_3/L$
Total inorganic carbon	c_T	mole/L
Bottom algae biomass	a_b	mgA/m^2
Bottom algae nitrogen	IN_b	mgN/m^2
Bottom algae phosphorus	IP_b	mgP/m^2
Constituent i		
Constituent ii		
Constituent iii		

MASS BALANCE



$$\frac{dc_i}{dt} = \frac{Q_{i-1}}{V_i} c_{i-1} - \frac{Q_i}{V_i} c_i - \frac{Q_{ab,i}}{V_i} c_i + \frac{E'_{i-1}}{V_i}\left(c_{i-1} - c_i\right) + \frac{E'_i}{V_i}\left(c_{i+1} - c_i\right) + \frac{W_i}{V_i} + S_i$$

$$\frac{da_{b,i}}{dt} = S_{b,i}$$

PHYTOPLANKTON AND DETRITUS STOICHIOMETRY:
The “Redfield Ratio”

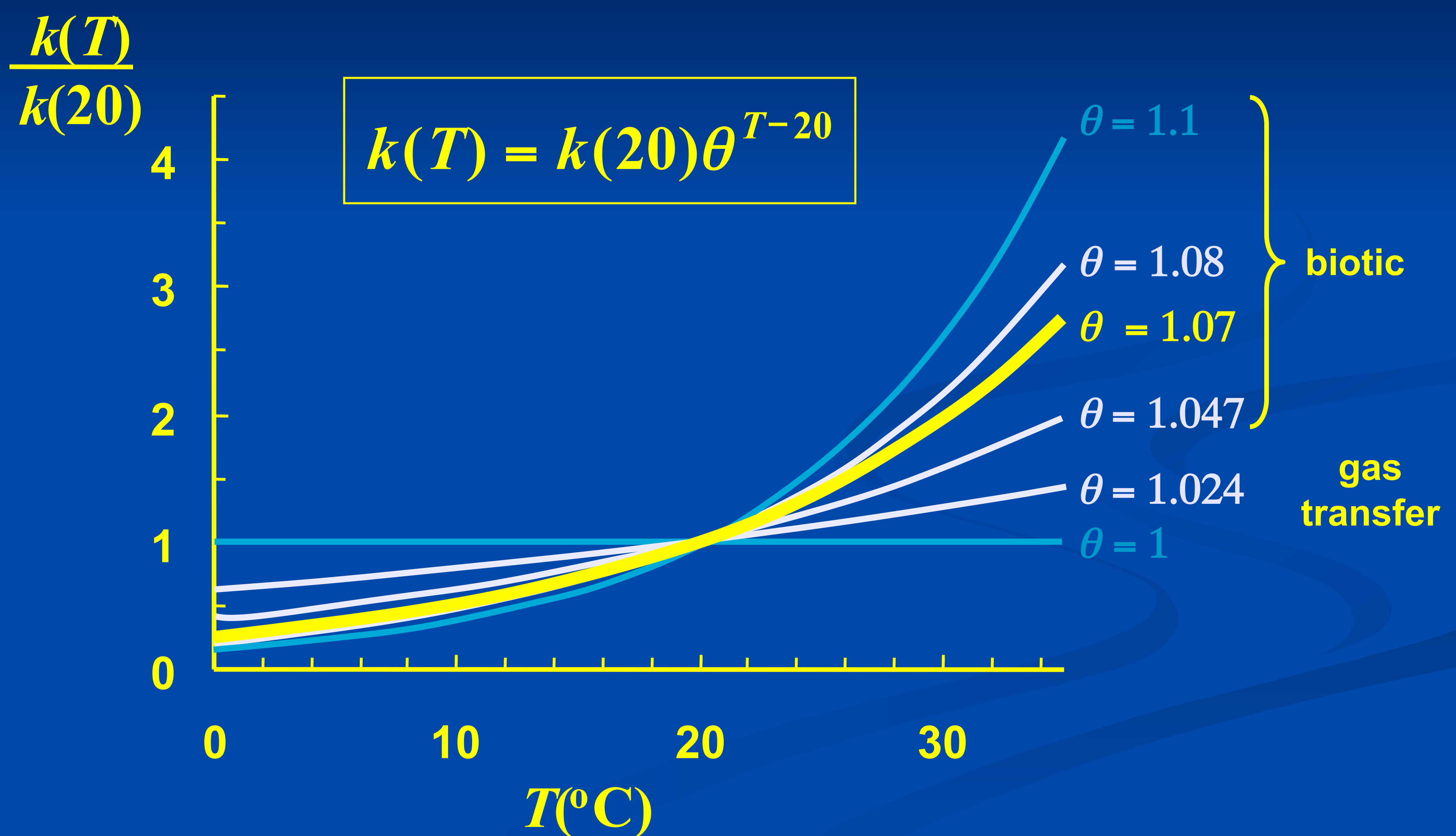
D	:	C	:	N	:	P	:	A
100%	:	40%	:	7.2%	:	1%	:	0.5-2.0%

	A	B	C	D
1	QUAL2K			
2	Stream Water Quality Model			
3	Streeter River (8/15/2002)			
4	Water Column Rates			
5				
6				
7	Parameter	Value	Units	Symbol
8	Stoichiometry:			
9	Carbon	40	mgC	
10	Nitrogen	7.2	mgN	
11	Phosphorus	1	mgP	
12	Dry weight	100	mgD	
13	Chlorophyll	1	mgA	

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

TEMPERATURE EFFECT ON THE REACTION RATE

$$k(T) = k(20)\theta^{T-20}$$



Q2K

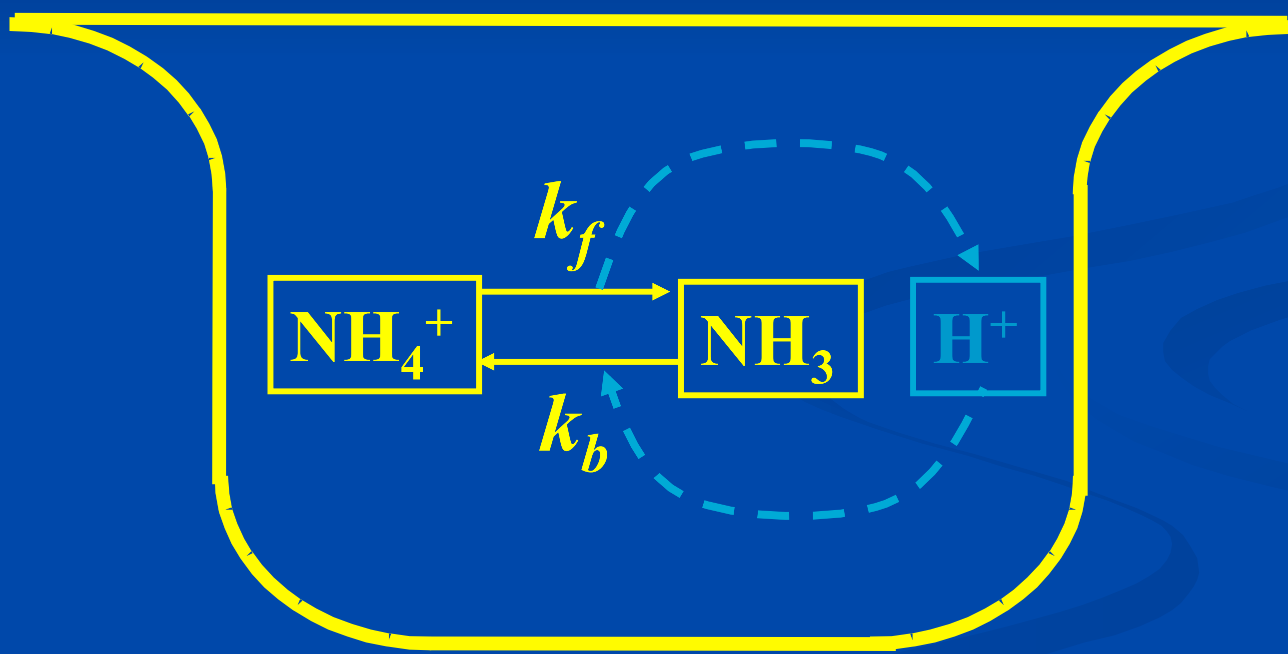
CHEMISTRY AND pH MODELING

- *Mass Balance versus Chemical Equilibria Models*
- *Chemistry 101*
- *Ammonia-Ammonium Acid Base*
- *pH Modeling*

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

THE CHEMISTRY PERSPECTIVE: AMMONIA ACID-BASE EQUILIBRIUM

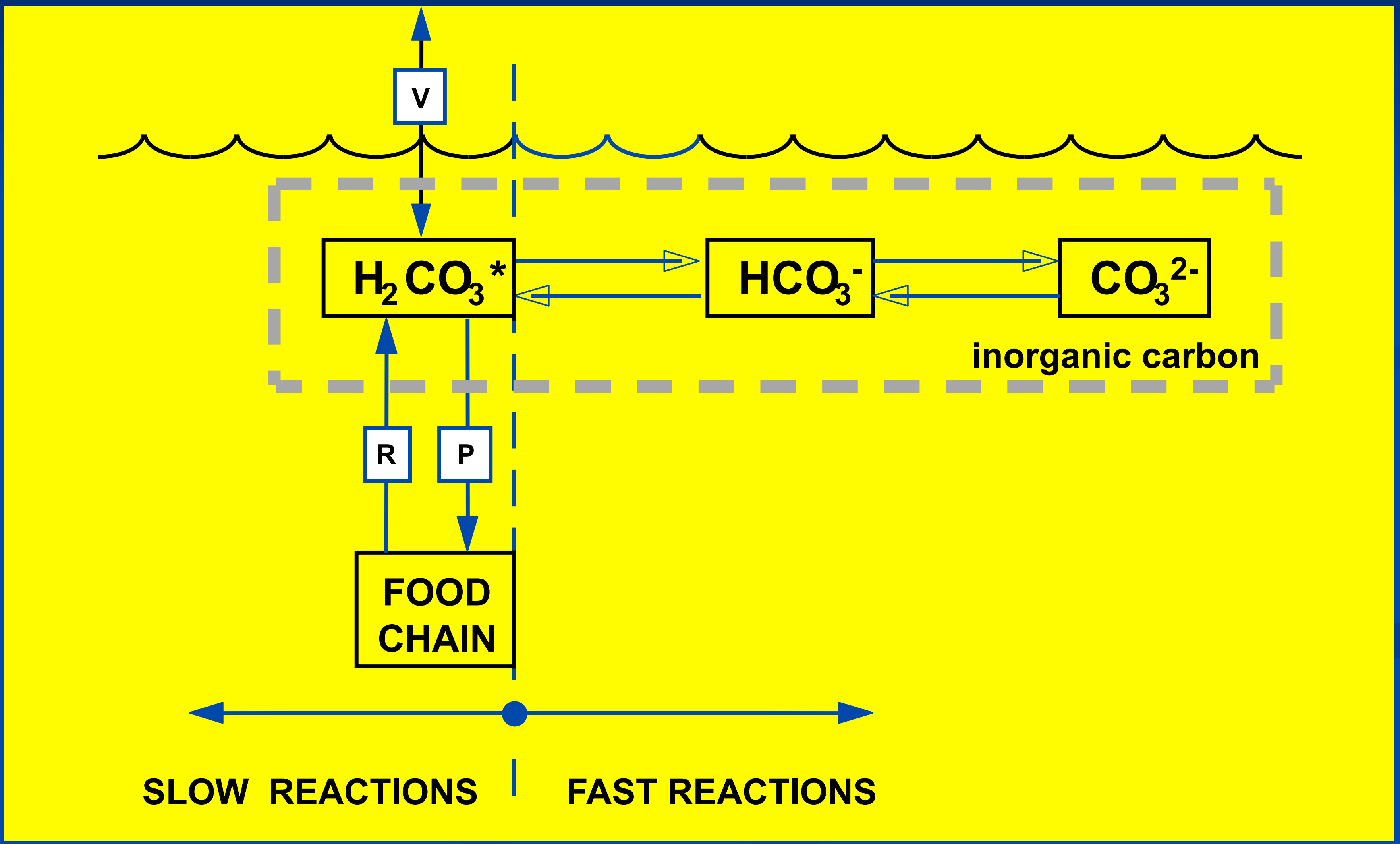
$$NH_4^+ \rightleftharpoons NH_3 + H^+$$



$$k_f[NH_4^+] = k_b[NH_3][H^+]$$

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

pH MODELING



Q2K PLANTS

- ***Phytoplankton***
- ***Stationary or Attached Plants***

Incorporating Limits to Growth

$$\frac{da}{dt} = k_g a$$

$$\text{if } a = a_0 \text{ at } t = 0$$

$$a = a_o e^{k_g t}$$

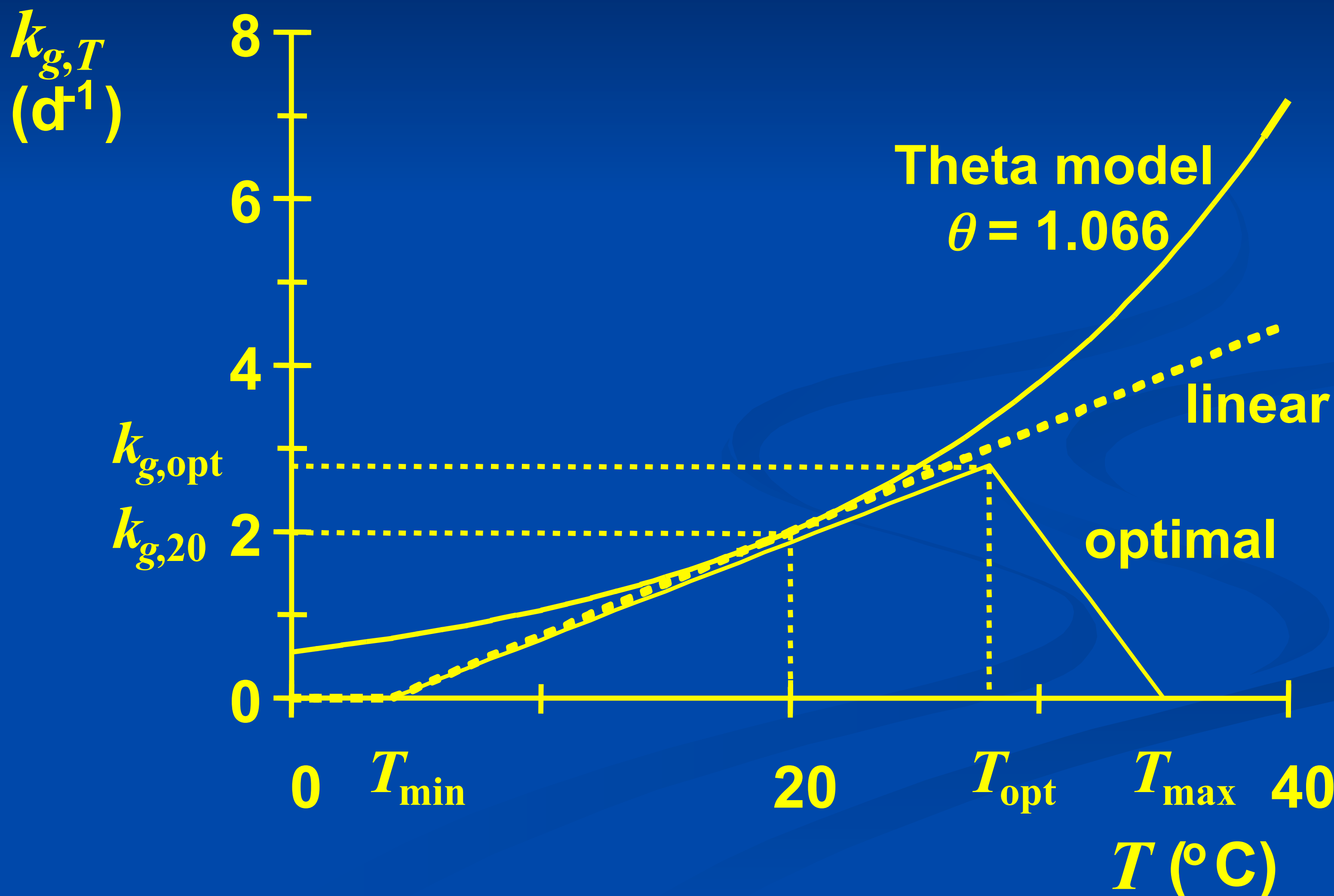
t, d	0	1	10	100
a, mg m^{-3}	1	7.8	4.85×10^{8}	7.2×10^{86}

$$\frac{da}{dt} = k_g(T, N, I)a - k_d a$$

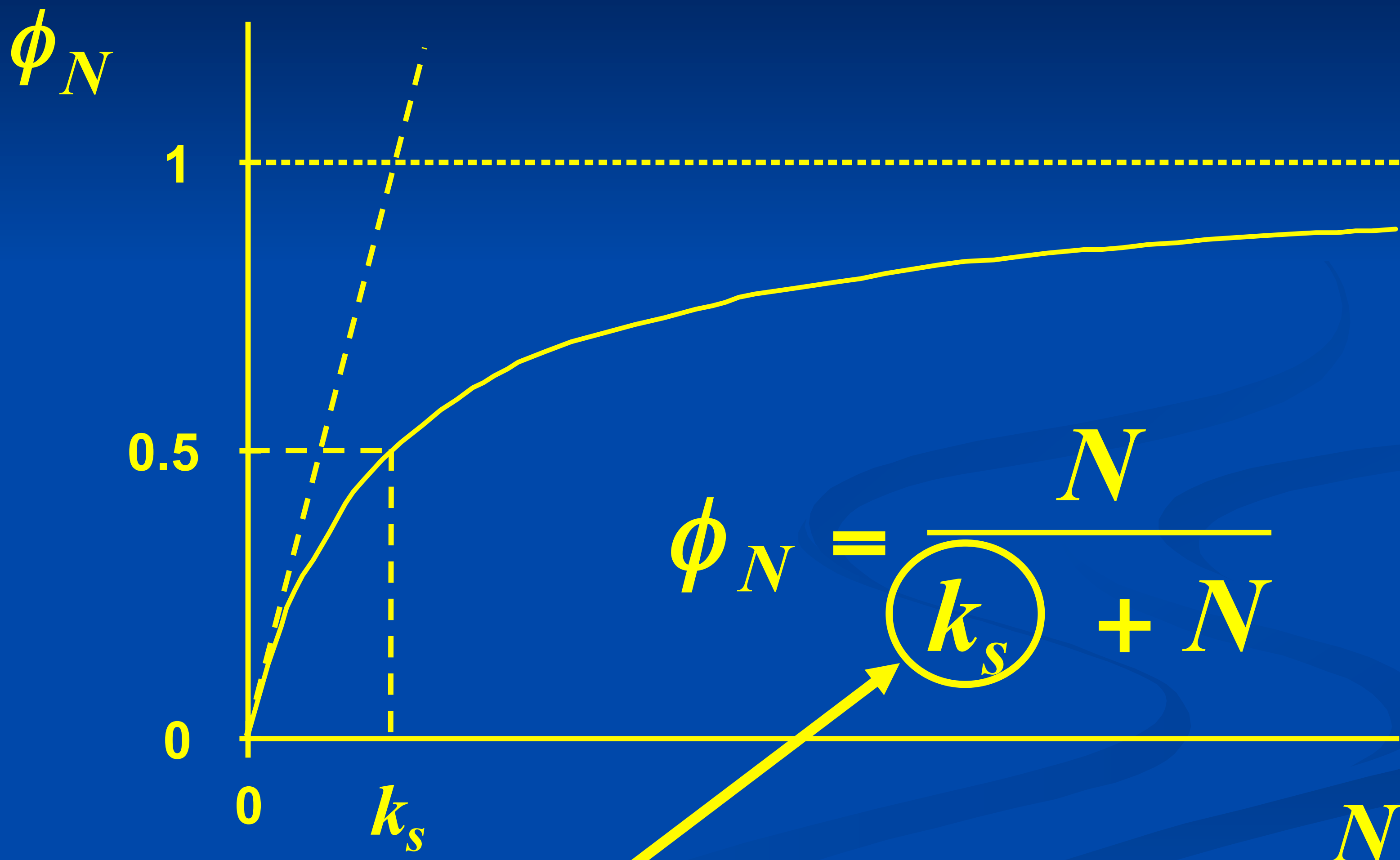
$$k_g(T, N, I) = k_{g,T}\phi_N \phi_L$$

temperature nutrients light

TEMPERATURE DEPENDENCY



NUTRIENT LIMITATION
MICHAELIS-MENTEN KINETICS



$$\phi_N = \frac{N}{k_s + N}$$

Half-saturation Constant

Light Response Models for Plant Growth

Saturation (Michaelis-Menten) Model:

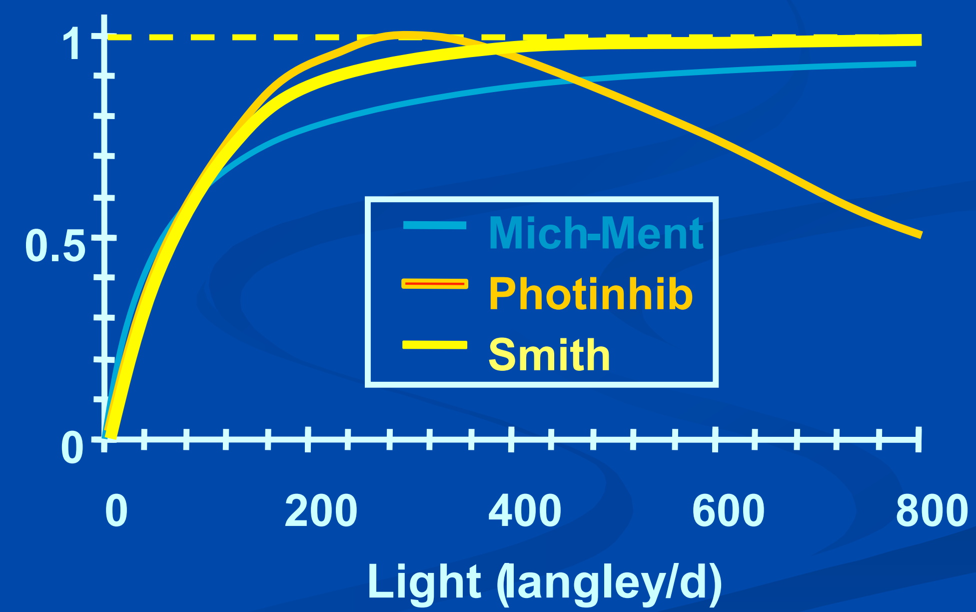
$$\phi_\ell = \frac{I}{k_{si} + I}$$

Photoinhibition Model:

$$\phi_\ell = \frac{I}{I_s} e^{1 - \frac{I}{I_s}}$$

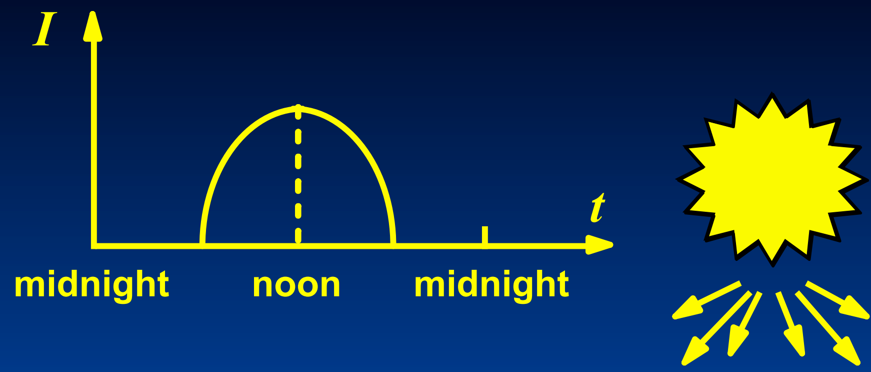
Smith Model:

$$\phi_\ell = \frac{I}{\sqrt{I^2 + I_k^2}}$$

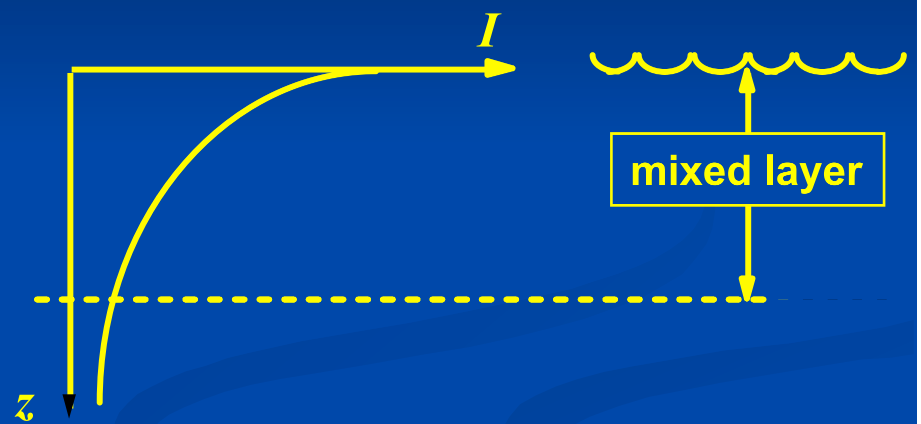


IMPACT OF LIGHT ON PHOTOSYNTHESIS

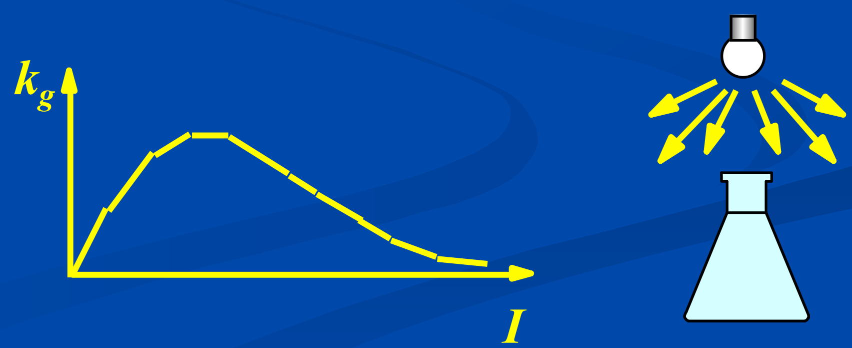
(*a*) Diurnal variation of light



(*b*) Light attenuation with depth



(*c*) Dependence of growth rate on light



STATIONARY OR "ATTACHED" PLANTS

- *Overview*
- *Simple Periphyton Modeling*
- *Macrophytes*

Differences between fixed and floating plants

	Floating	Attached
Transport	Yes	No
Types	Diatoms Greens Blue Greens	Periphyton Filamentous Algae Rooted Macrophytes
Units	mgchl a/m^3	gD/m^2 or mgA/m^2
Light	Average Water Column	Bottom Light
Predation	Zooplankton	Insect Larvae, Snails, etc.
Substrate	Not an issue	Rock vs. Mud

Functional Groups

- **Periphyton: algae attached to and living upon submerged solid surfaces**
  - **Diatoms, Greens, Blue Greens**
- **Filamentous Algae**
  - **Cladophora**
- **Macrophytes: Vascular, Rooted Plants**
  - **Myriophyllum, Elodea, Potamogeton**

PERIPHYTON MODELS

Based on integral light

Phytoplankton:

$$\frac{da_p}{dt} = k_g(T)\phi_l \phi_n a_p - k_r a_p - k_d a_p + transport\text{ - }settling$$

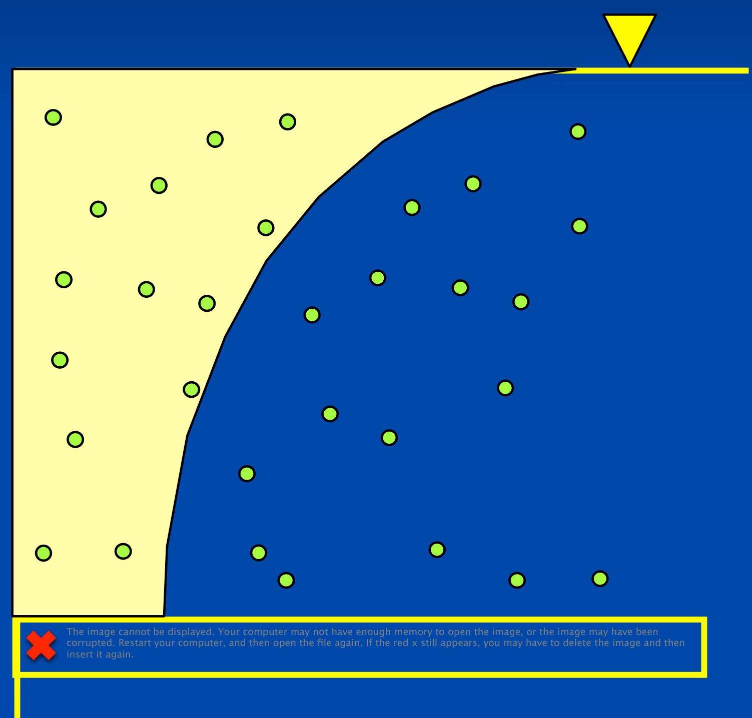
Based on bottom light

Periphyton:

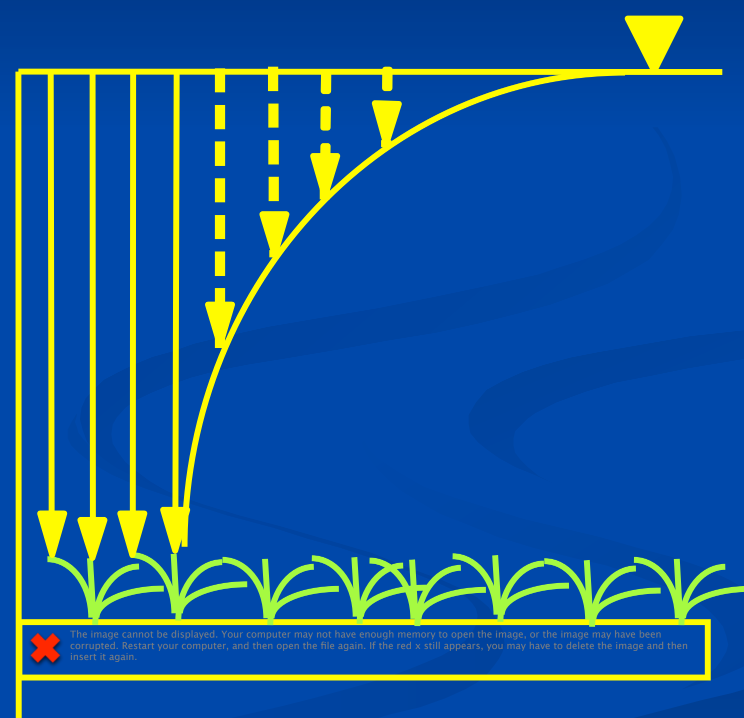
$$\frac{da_f}{dt} = G_{max}(T)\phi_l \phi_n - k_r a_f - k_d a_f$$

Developed by Steve Chapra for 2004 QUAL2K Workshop (Some slides have been updated)

EFFECT OF LIGHT ON PERIPHYTON



(*a*) floating plants



(*b*) periphyton

Macrophytes

- Vascular, Rooted Plants
- Myriophyllum, (Water milfoil) Elodea, (Waterweed) Potamogeton (Pondweed Oxygen weed)
- Lakes/Slow-moving streams/shallow rivers
- Can extend up into water column
- Can get nutrients from roots

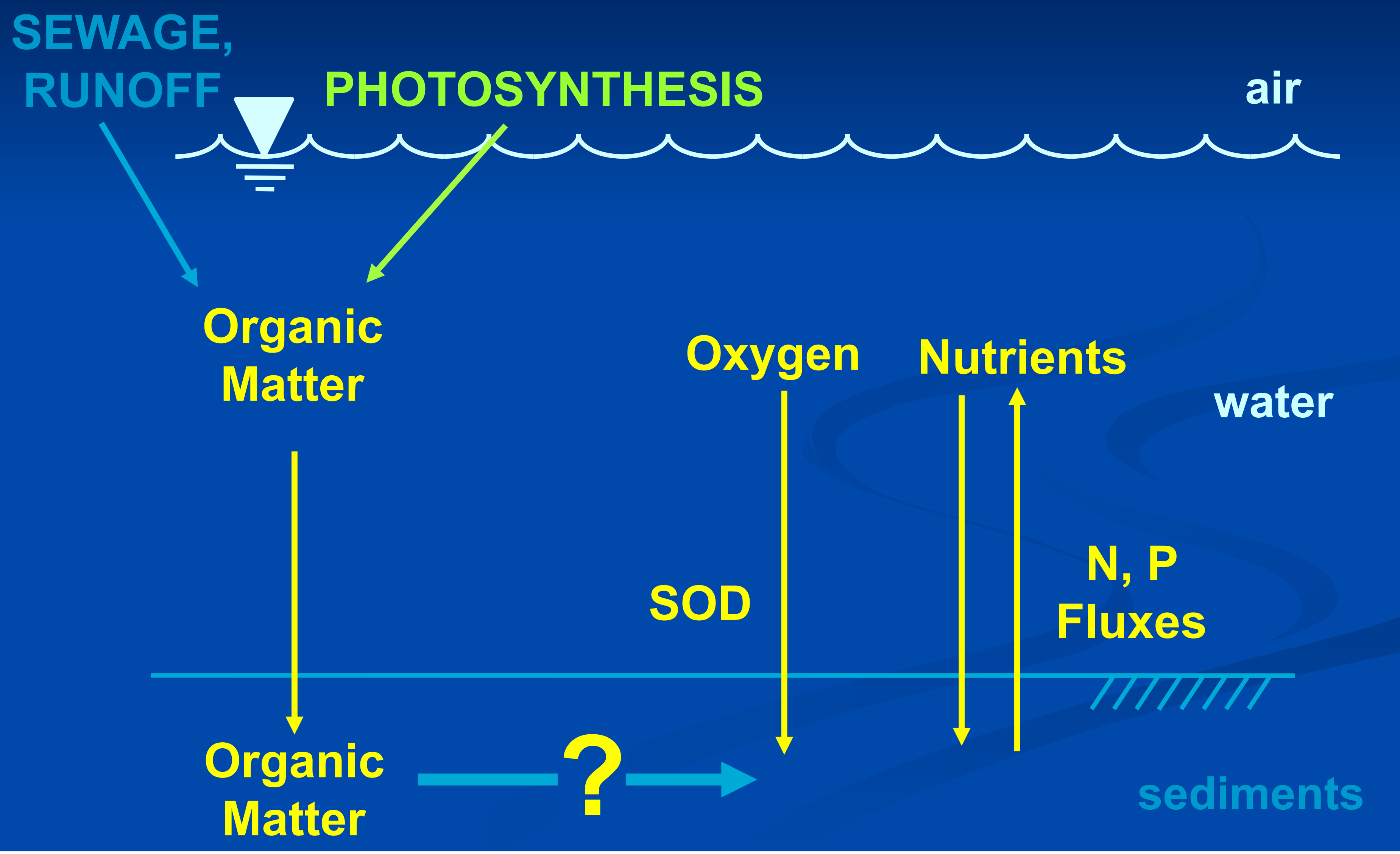
Q2K

SEDIMENT/WATER INTERACTIONS

- *Sediment Oxygen Demand*
- *Methane Bubble Formation*
- *Diffusion/Reaction Competition*
- *Numerical Methods*

SEDIMENT-WATER PROCESSES

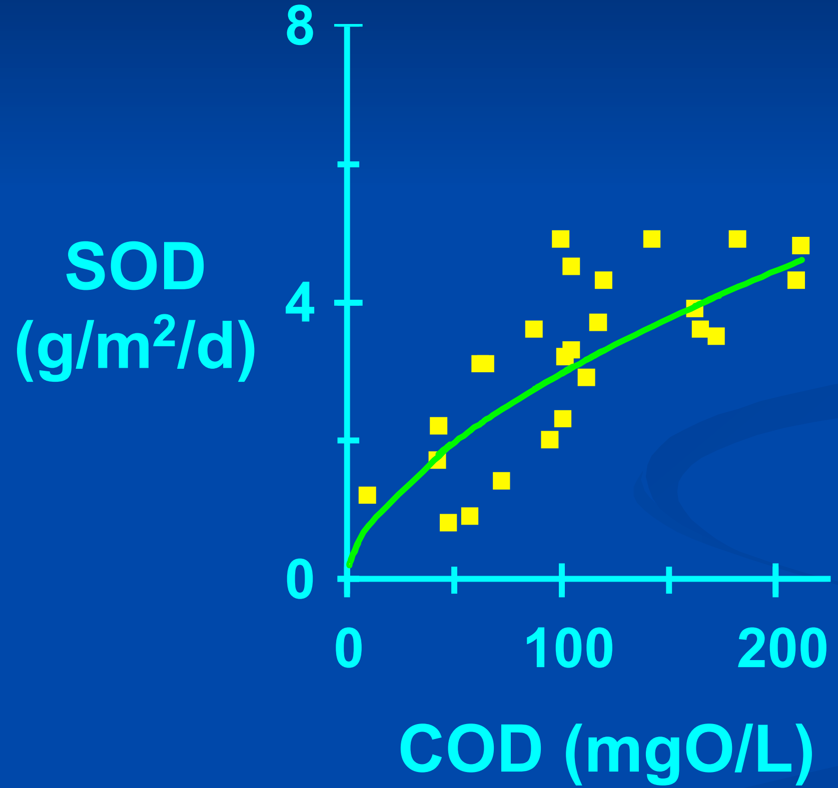
"THE MISSING LINK OF WATER-QUALITY MODELLING"



TYPICAL SOD VALUES

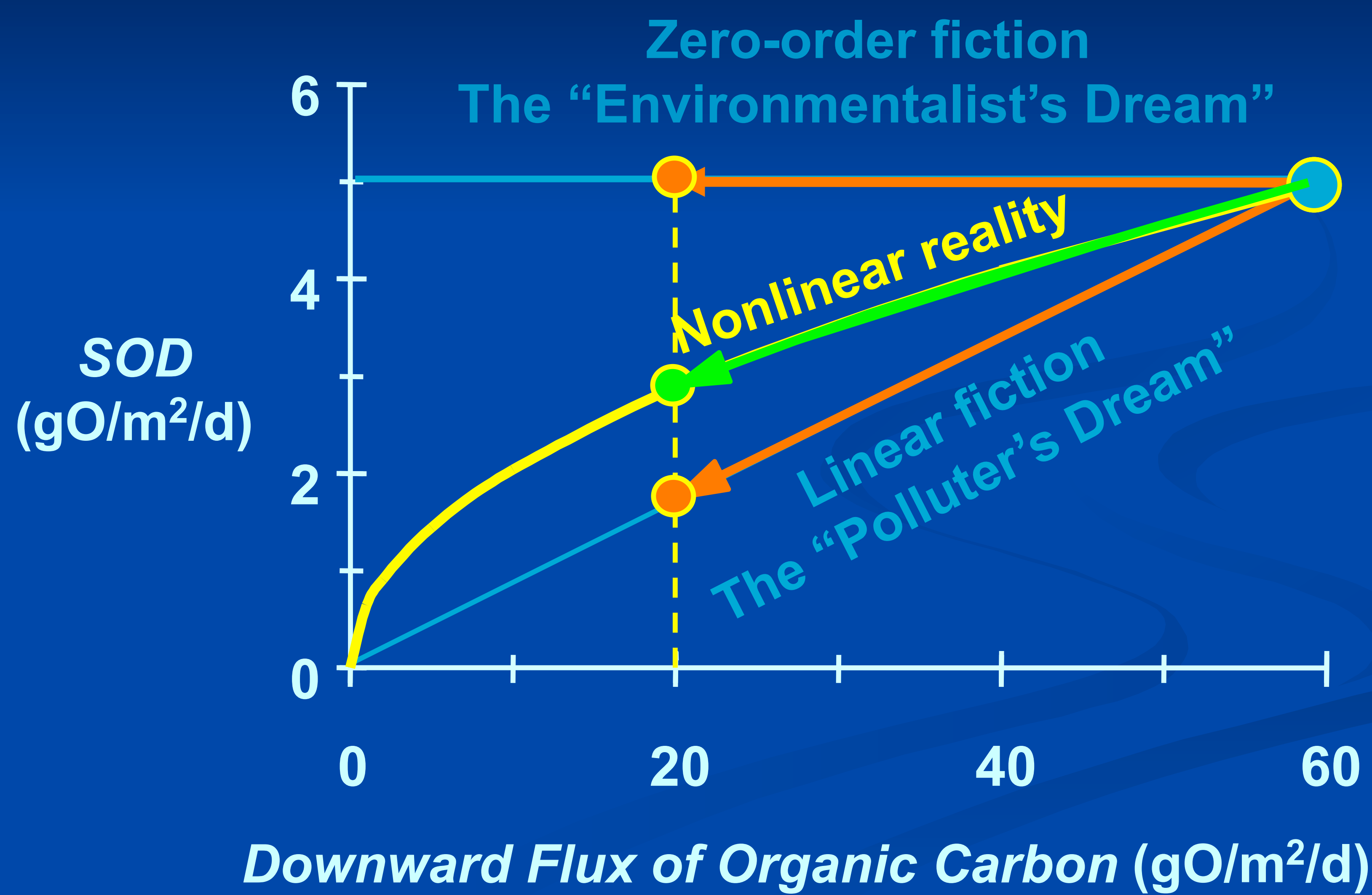
	$S'_{B,20}$ (g m^{-2} d^{-1})	
Bottom type and location	Average value	Range
Sphaerolitus (10 g dry wt/m^2)	7	-
Zebra Mussels (6000 individuals/m^2)	5	-
Municipal sewage sludge		
outfall vicinity	4	2-10
downstream of outfall, "aged"	1.5	1-2
Estuarine mud	1.5	1-2
Sandy bottom	0.5	0.2-1
Mineral soils	0.07	0.05-1
Areal hypolimnetic oxygen demand (AHOD) -- lakes		0.06-2

THE "SQUARE-ROOT" RELATIONSHIP OF SEDIMENT OXYGEN DEMAND AND OVERENRICHMENT



$$SOD = \alpha \, COD^{0.5}$$

WHY NONLINEARITIES MATTER



WHERE DOES NONLINEARITY COME FROM?

- **Loss of carbon as methane gas in anaerobic sediments**
- **Competition between reaction and diffusion in aerobic surface sediment**

CALIBRATION

- Seems like a lot of parameters
- *For steady state*, really only three
  - Mass transfer, v_{d01}
  - Reaction rates, $k_{n1} + k_{c1}$

New QUAL2KW Versions

- **Available from Washington Ecology:**
  - **http://www.ecy.wa.gov/programs/eap/models.html**
- **Version 5**
  - **Repeating diel simulation**
  - **Updated user manual**
- **Version 6**
  - **Kinematic wave flow routing**
  - **Fully dynamic for flow and other boundary conditions up to 365 days**

QUAL2K

Boulder Creek Example available in Q2K version 2_11b8

Modified for Region 6 Modeling Workshop, November 2013, by Robert Ambrose

Boulder Creek Example

- *Create a folder:* **C:/Q2K**
- *Unzip* **Q2K*.zip** *in this folder*
- *Files* **Q2KMaster*.xls** *and* **q2kfortran*.exe** *should be in this folder*
- *Create a folder:* **C:/Q2K/DataFiles**

Boulder Creek Example

- *Launch* **Q2KMaster.xls**
- *Change* **Saved File Name**
  to **Boulder Creek**
- *Change* **Directory where file stored**
  to **C:/Q2K/DataFiles**
- *Click* **Run Fortran** *button*