Project no.: 511254 (STREP)

SEDBARCAH

SEDiment BioBARriers for
Chlorinated Aliphatic Hydrocarbons
in ground water reaching surface water

CAH-Modeling & Batch & Column Tests (Part III)

Harald Kalka

Short Lecture at the Meeting
Leuven, January 2007

Start date of project: 01/01/2005 Duration: 2 years
Lead contractor for Work Package 5 (Modeling): UIT GmbH Dresden

CAH-Modeling

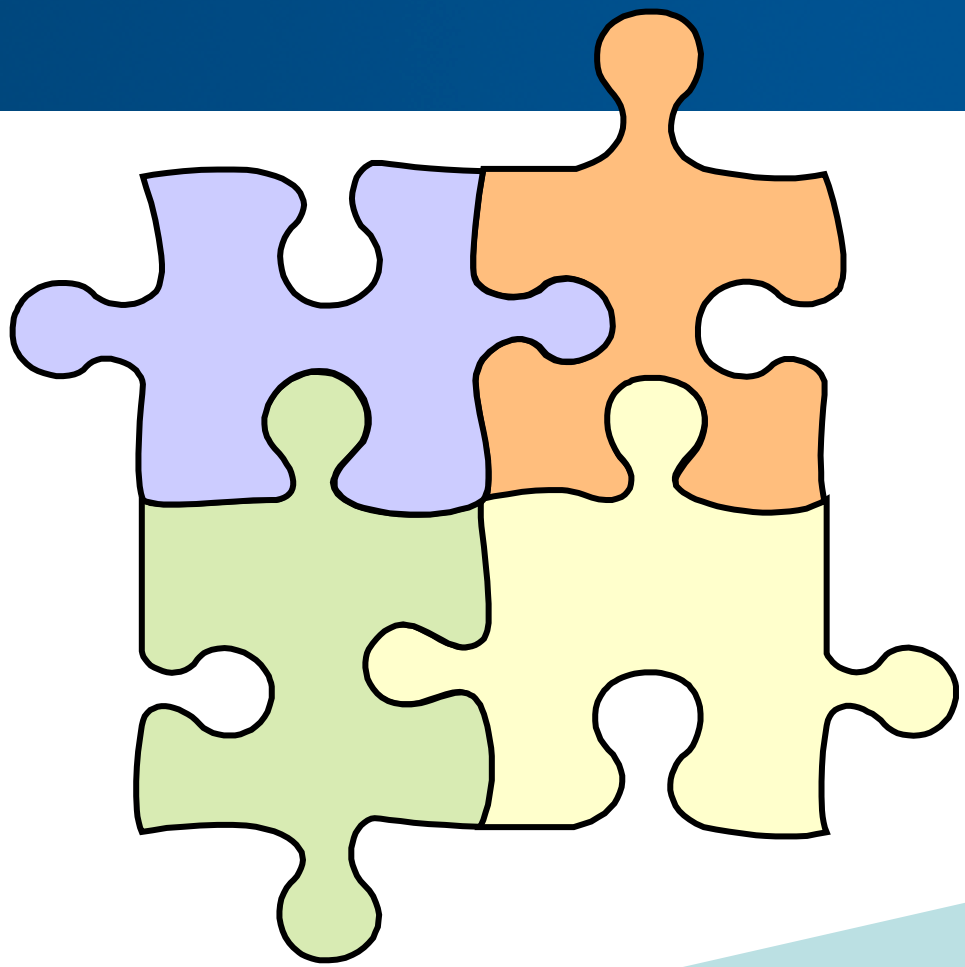
SEDBARCAH

1. Basic Idea
2. DCE & VC degradation
3. The Complete Chain
4. Column Tests
5. Conclusions & Outlook

The D13 Puzzle

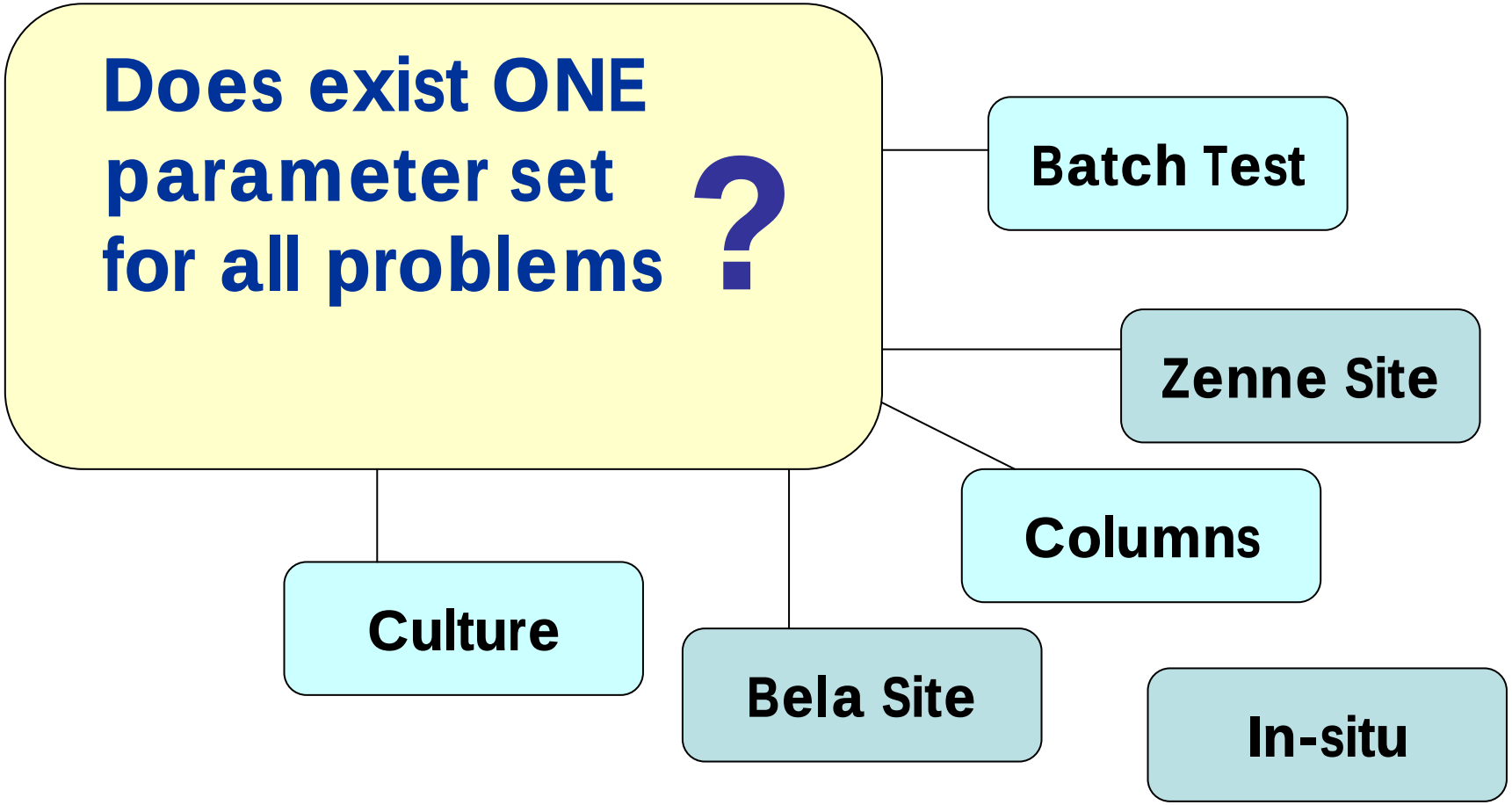
A huge number of experiments.

About 30 model parameters.

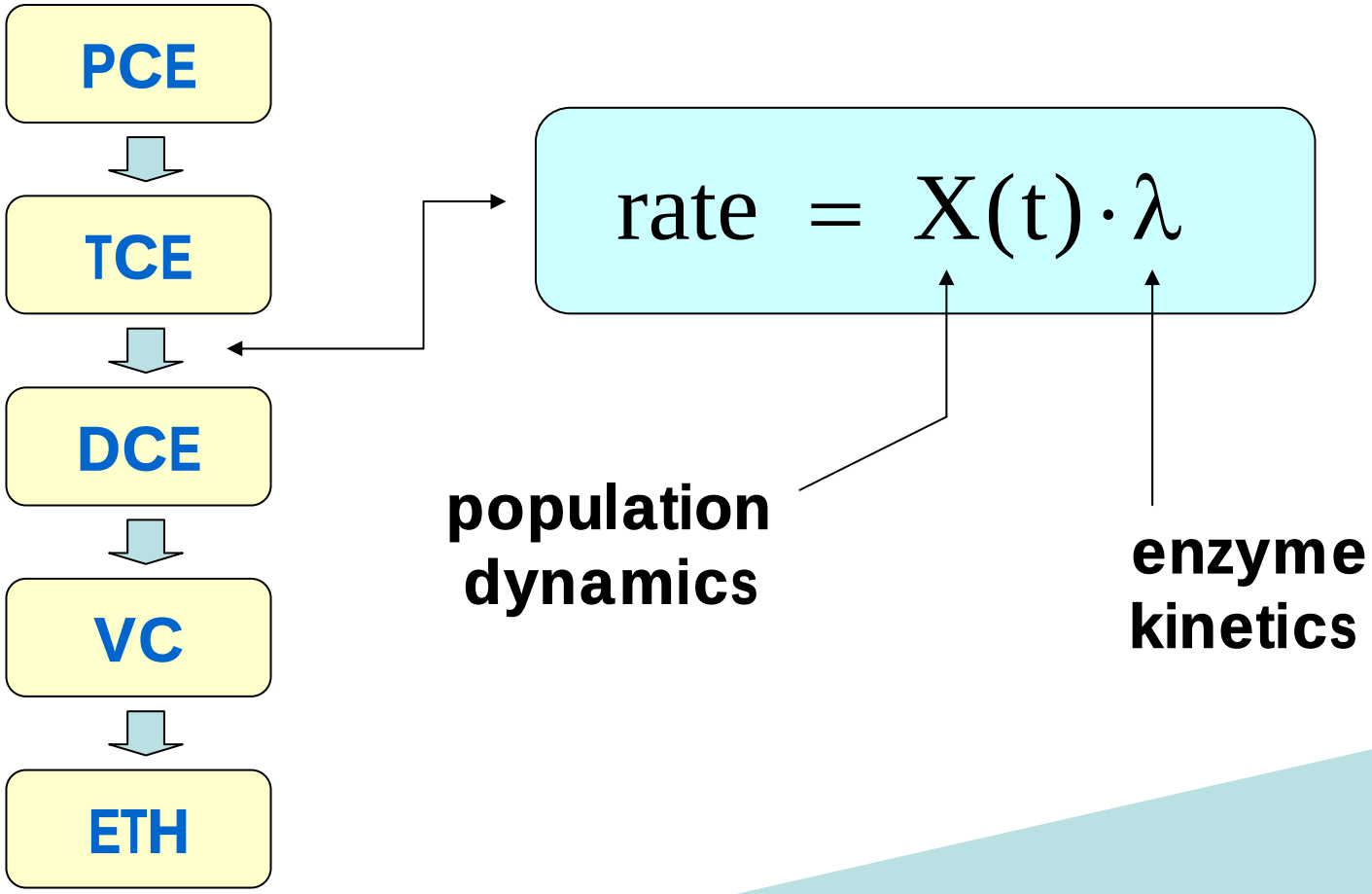


4 000 Calculations

Main Question



Basic Idea



Factorization Ansatz

Enzyme Kinetics

specific rate

$$\lambda_{i\to j} = \frac{k_i}{K_i\left(1+\frac{[i-1]}{K_{i-1}}+\frac{[i+1]}{K_{i+1}}\right)+[i]\left(1+\frac{[i]}{K_{ii}}\right)}$$

saturation

self-inhibition

3×4 Parameters

Kinetic Parameter Set

	k_i	K_i	K_{ii}
	µmol/µg/d	µM	µM
PCE	0.06	1.6	0
TCE	0.60	1.8	900
DCE	0.07	1.8	750
VC	0.008	5	750

pure culture

batch & column tests

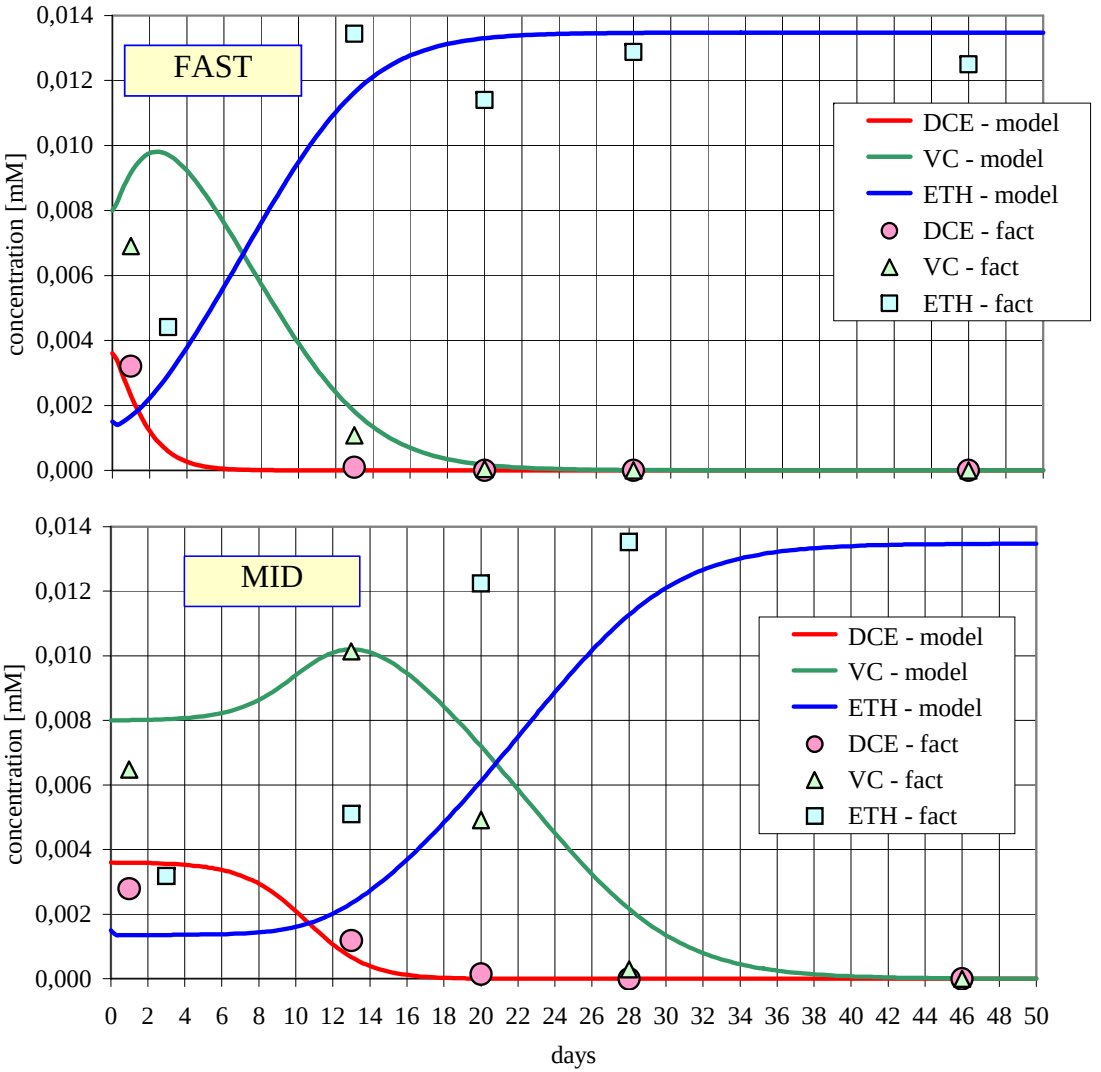
modified literature data

Zenne / DCE degradation

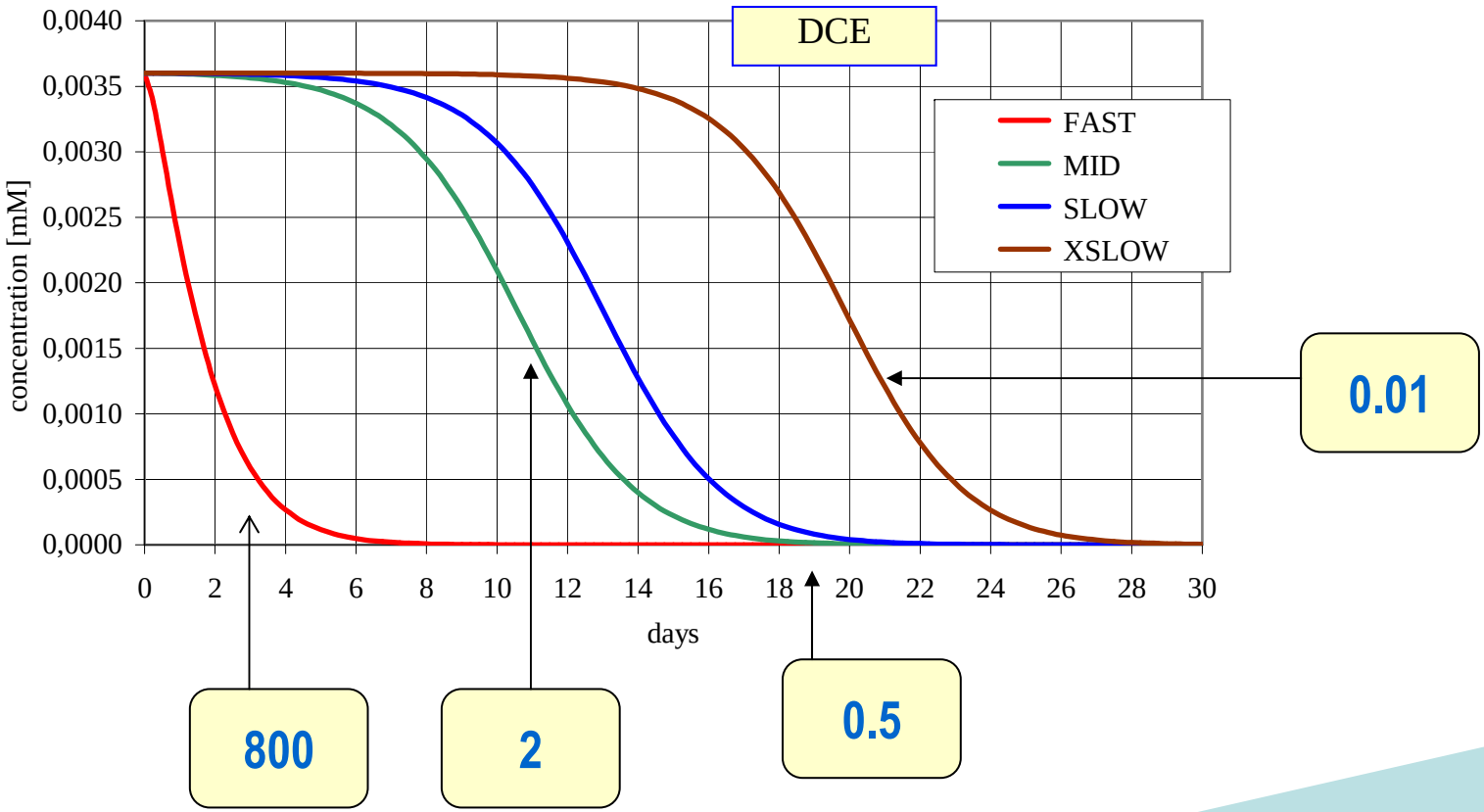
	initial population X_0
	µg/L pore water
FAST	800
MID	2
SLOW	0.5
xSLOW	0.01

all data bundled into 4 groups

fitted parameter



Variation of X_0



initial biomass in µg/L

CAH-Modeling

Population Dynamics

Zenne DCE

Bacterial Growth

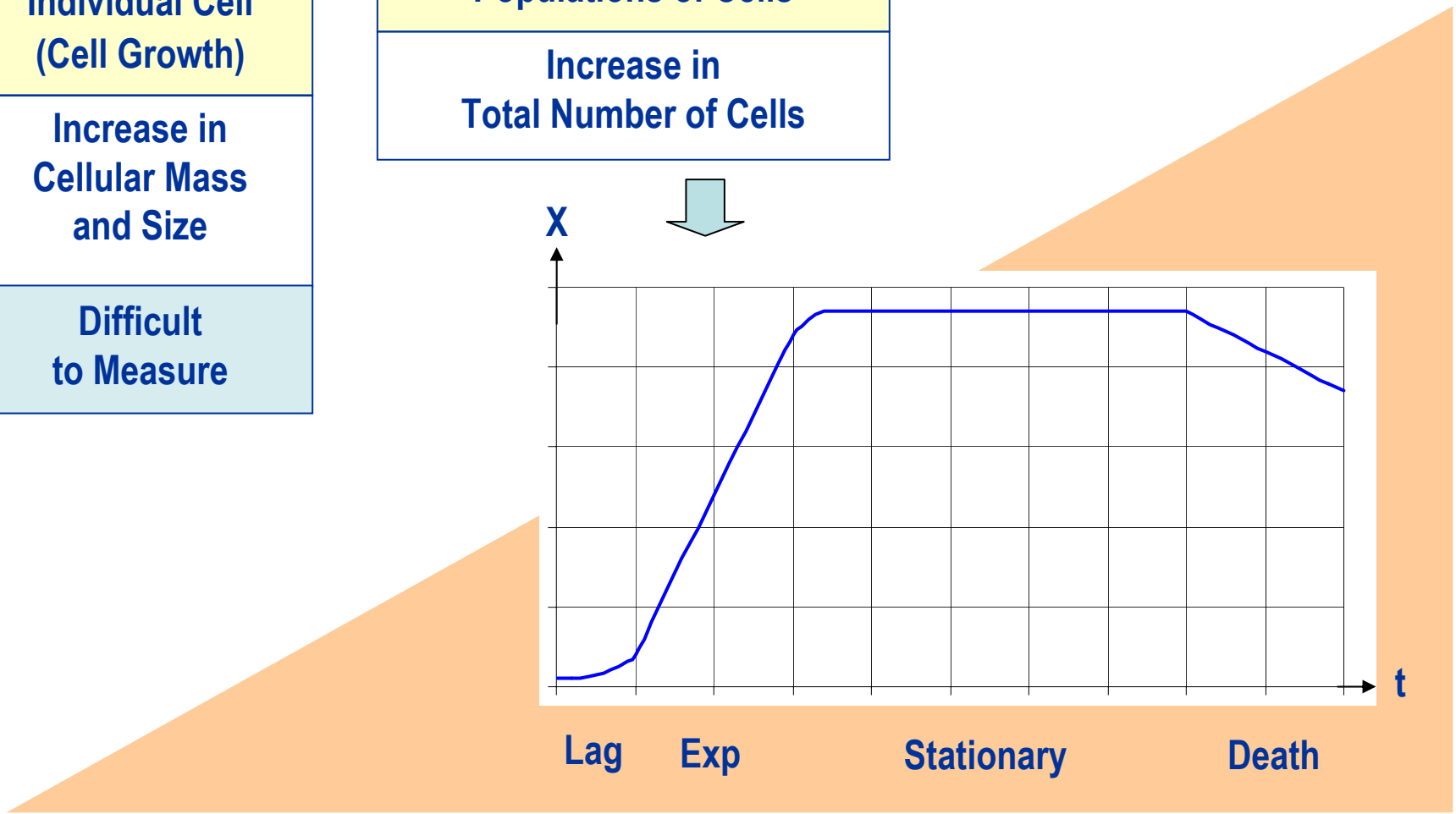
Individual Cell (Cell Growth)

Increase in Cellular Mass and Size

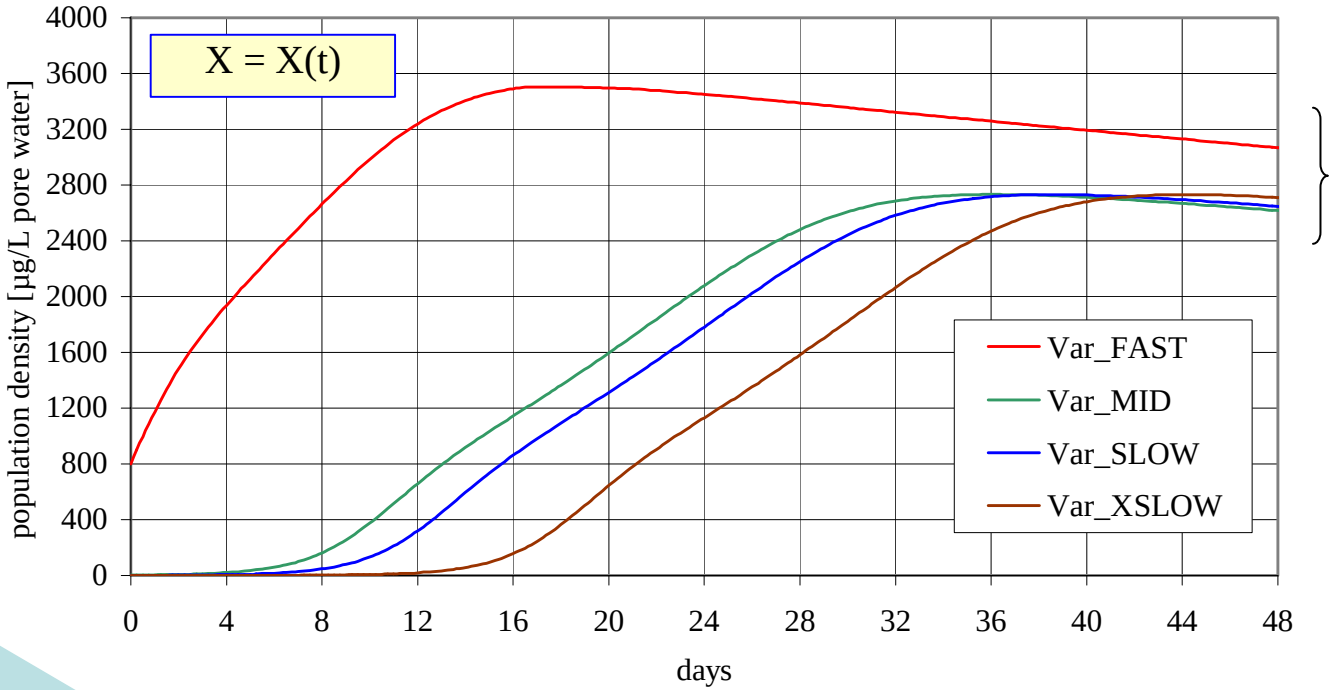
Difficult to Measure

Populations of Cells

Increase in Total Number of Cells



Population Growth for various X_0



yield

$$\frac{dX}{dt} = Y\Omega - \Gamma X$$

death rate

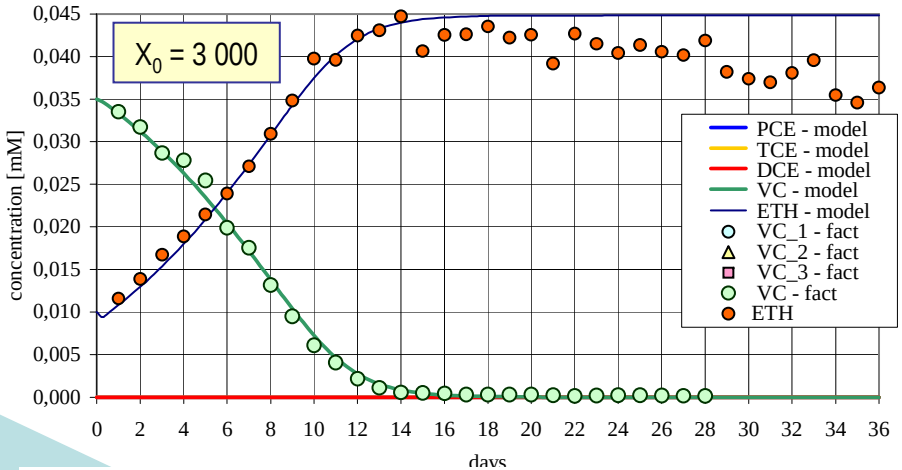
Zenne DCE

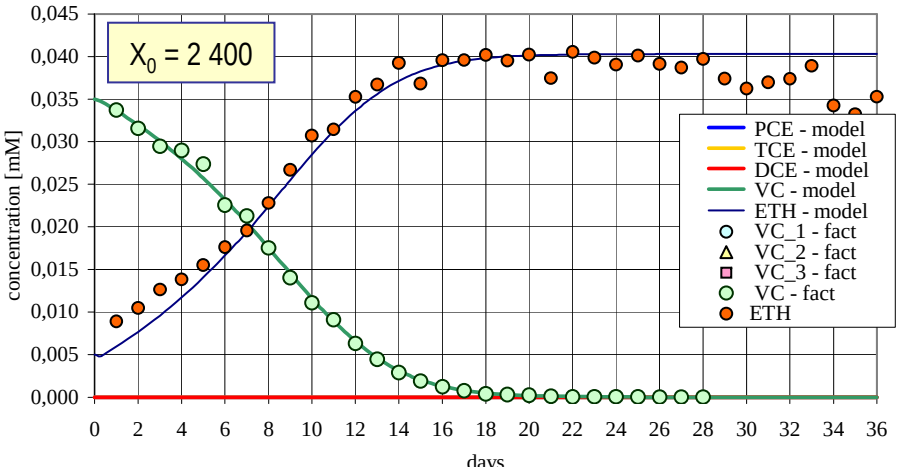
CAH-Modeling

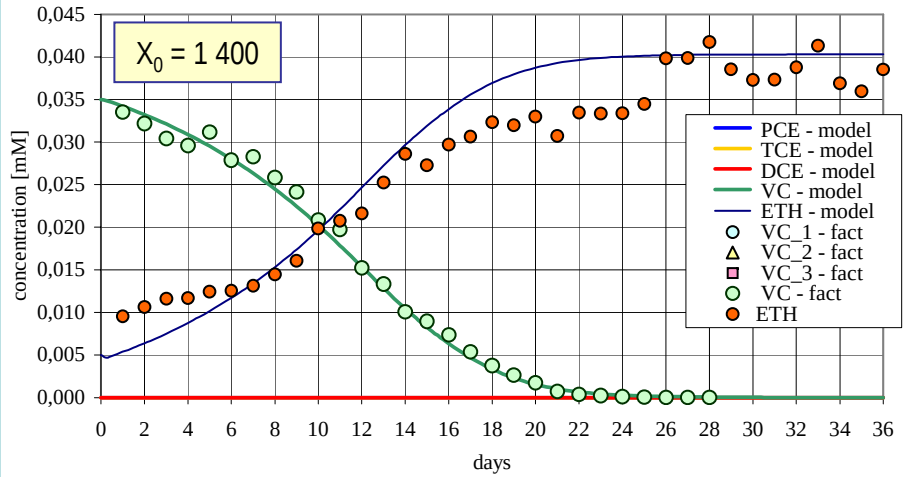
BATCH TEST

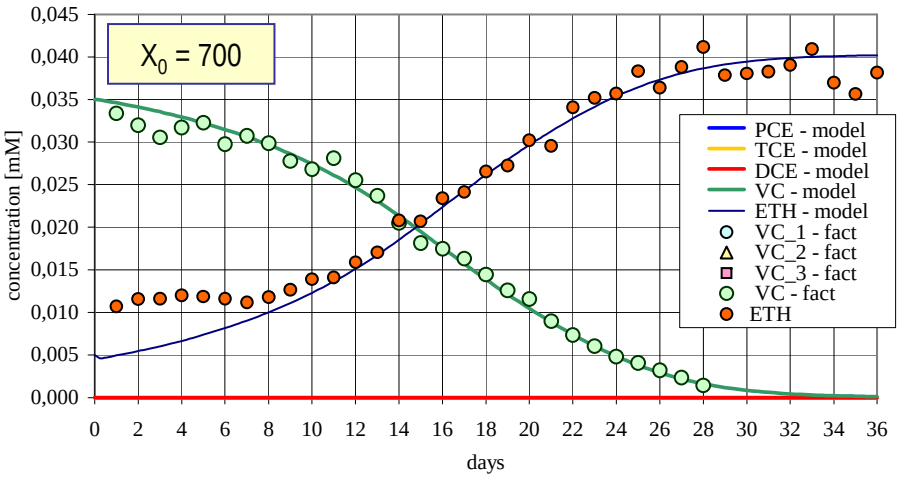
VC and DCE degradation

Zenne / VC Degradation





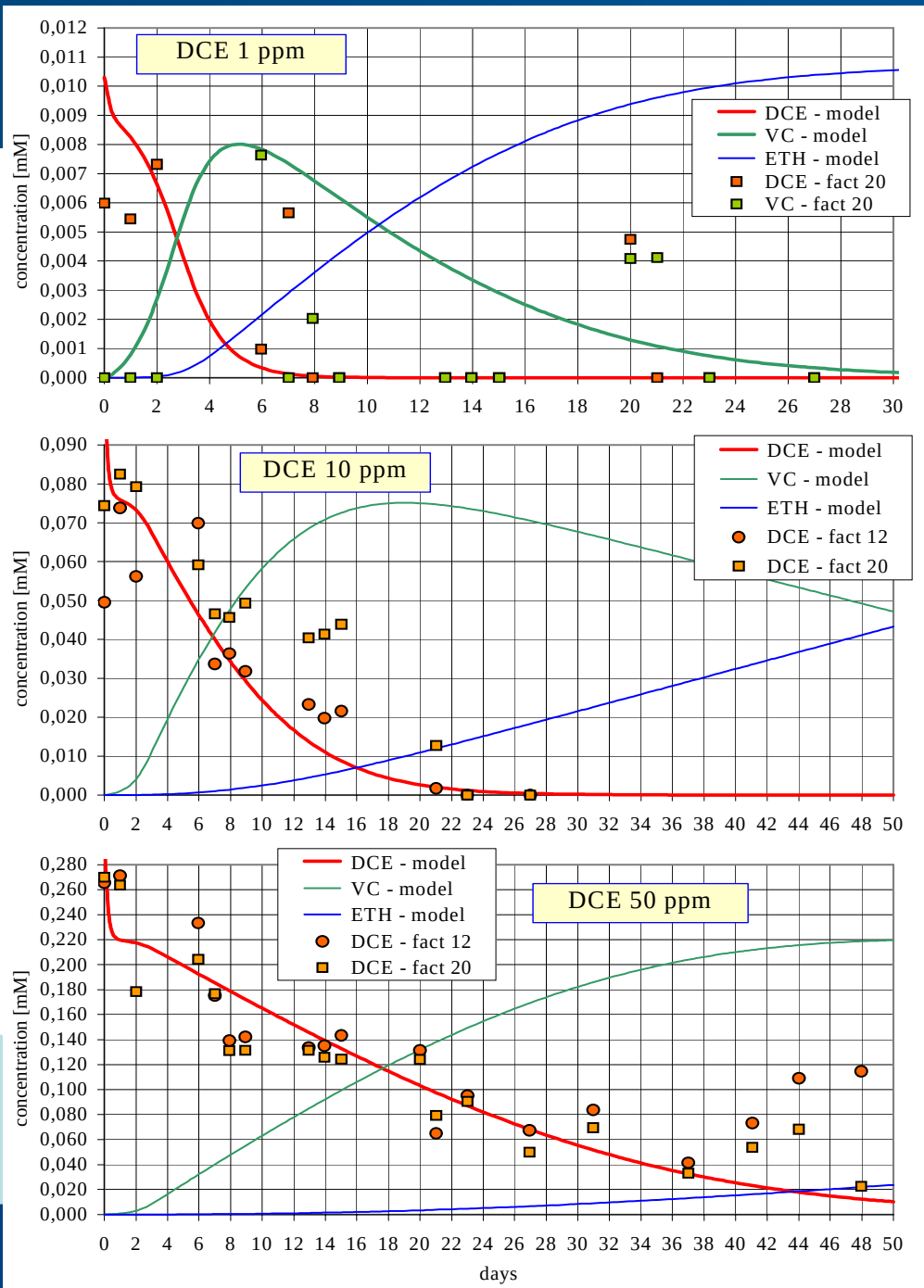




Bela Site

DCE degradation in sediment MP1

X_0 = 100 µg/L



CAH-Modeling

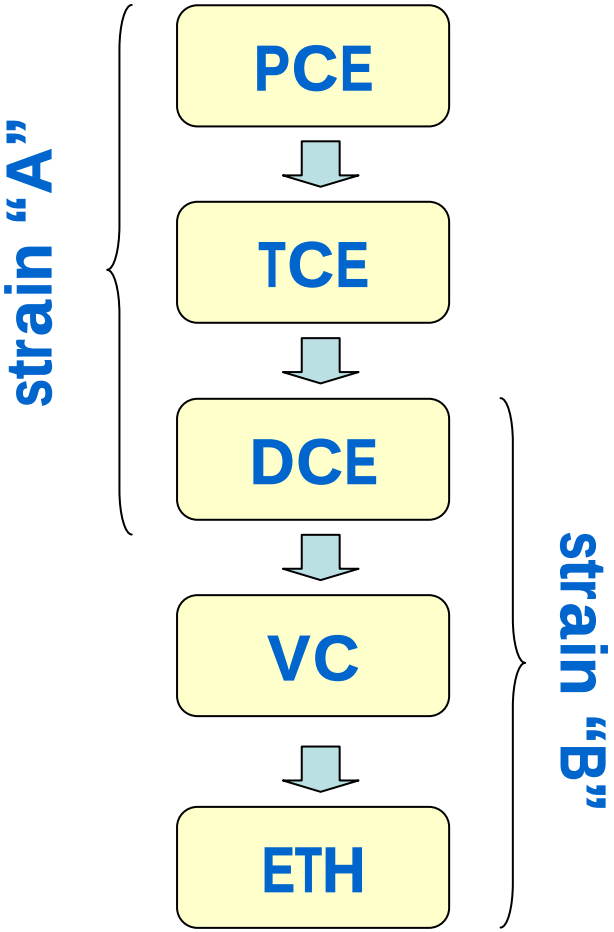
BATCH TEST

The complete degradation chain

PCE Degradation

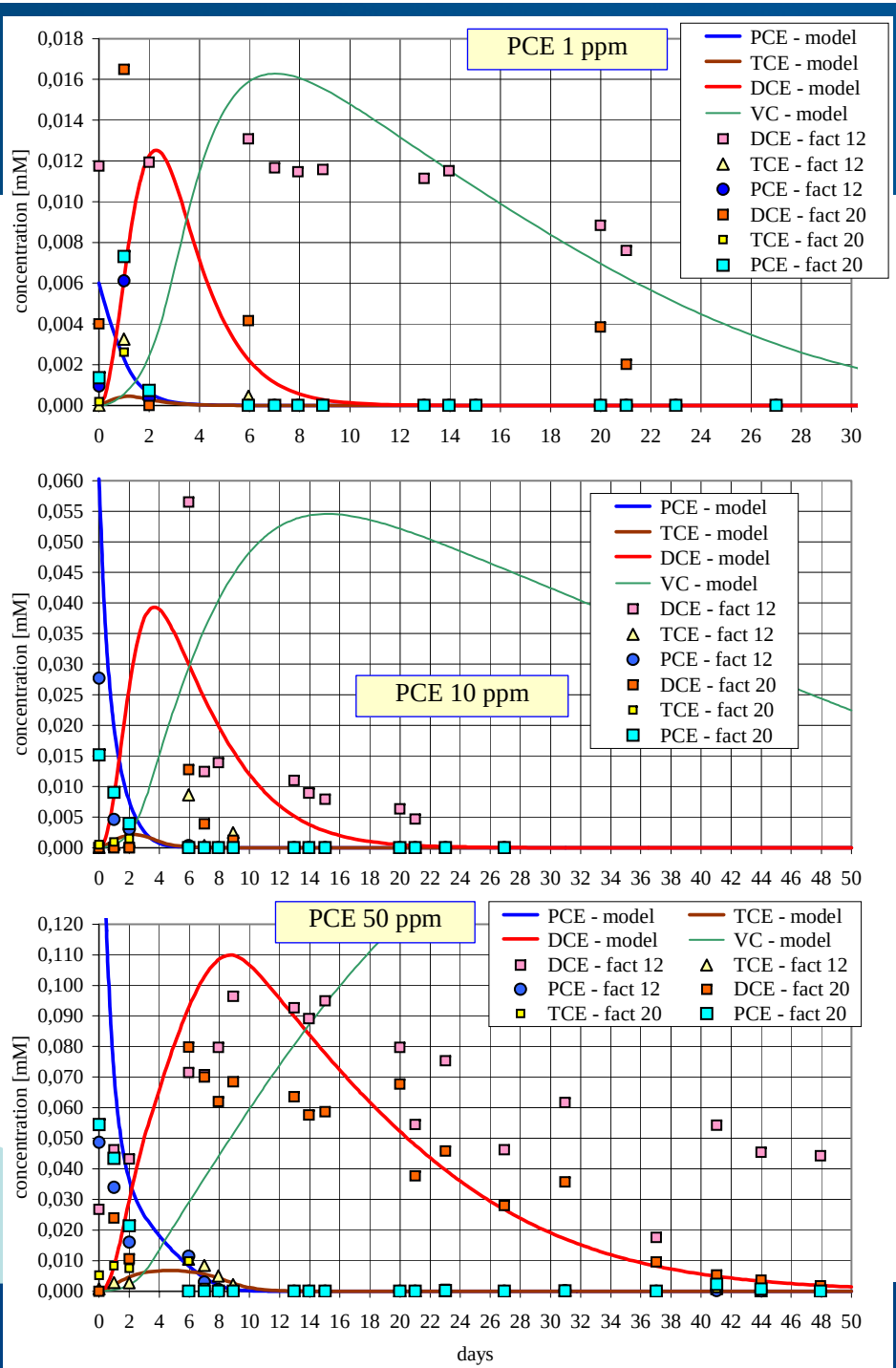
What is new ?

1	Strong Adsorption
2	Two Strains



Bela Site

PCE degradation in sediment MP1

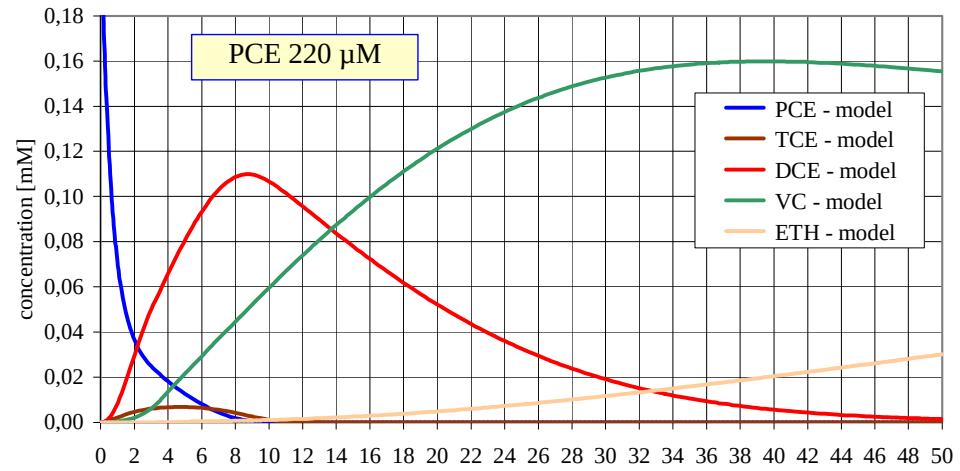


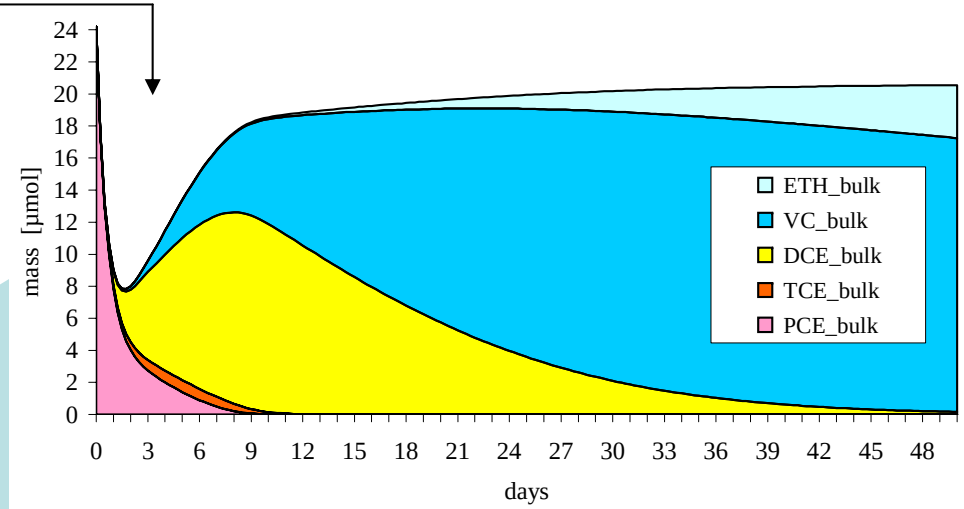
X_0 = 2 000 µg/L

January 2006

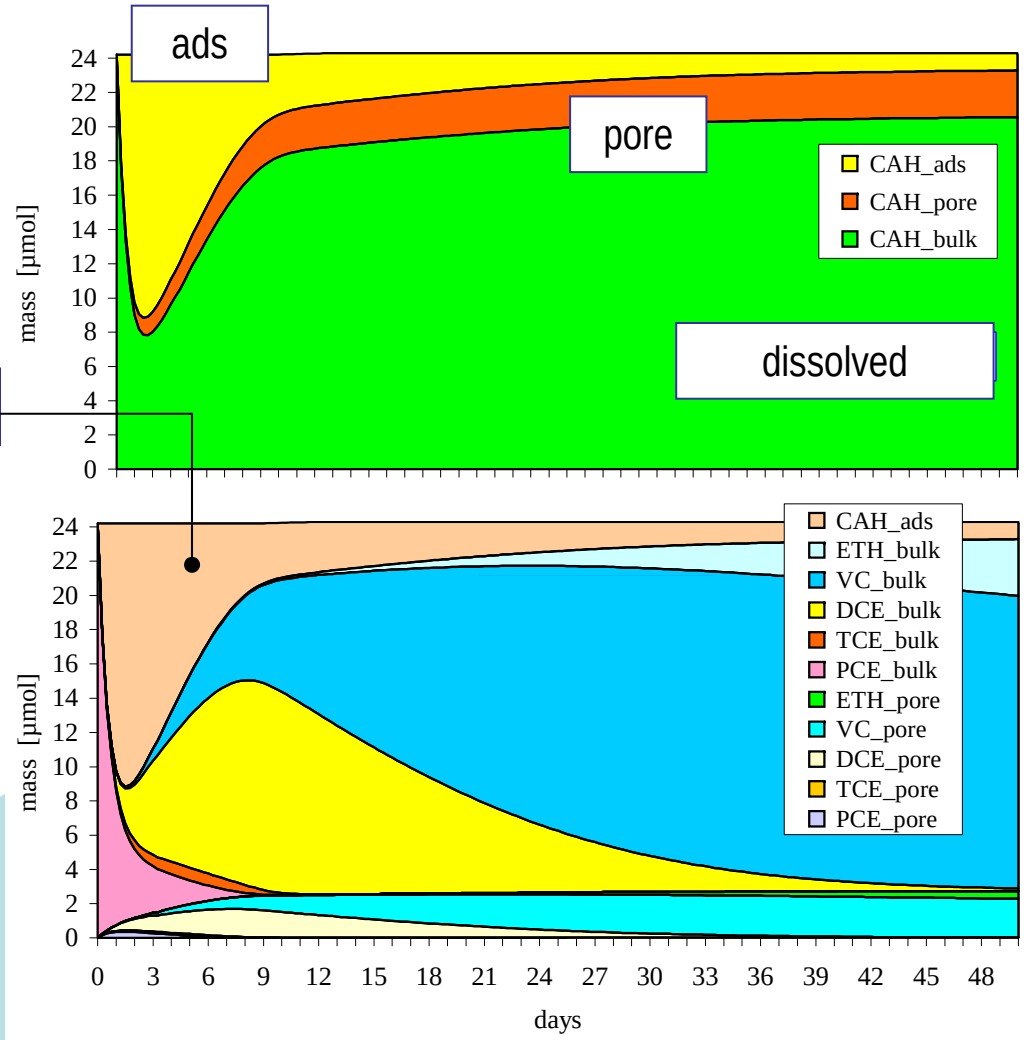
Ignoring Adsorption

Mass Balance Violation ?





Mass Balance for PCE Degradation

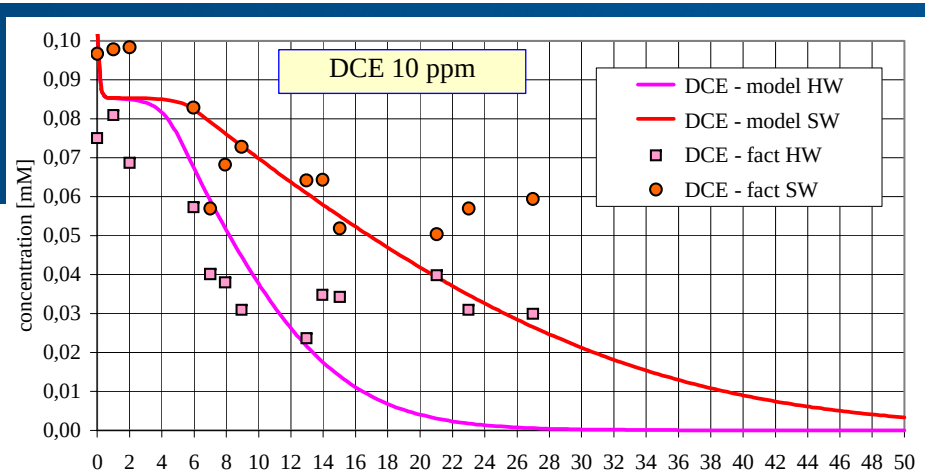


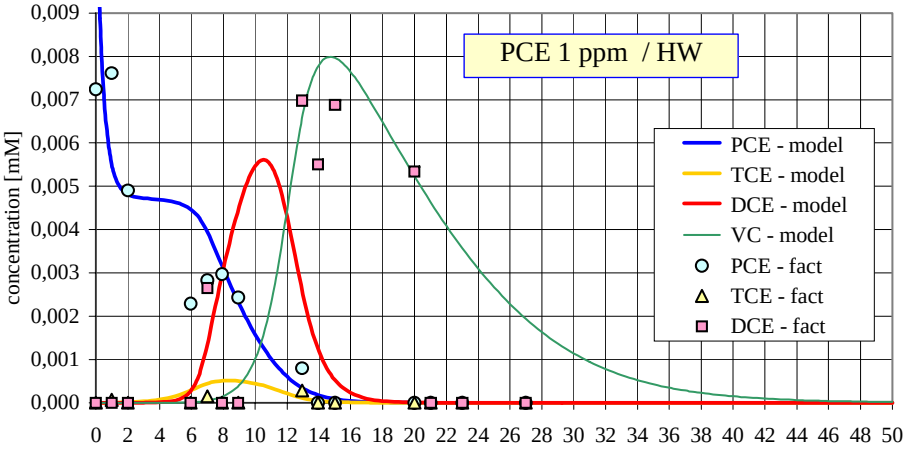
$$\sum m_i = \text{const}$$

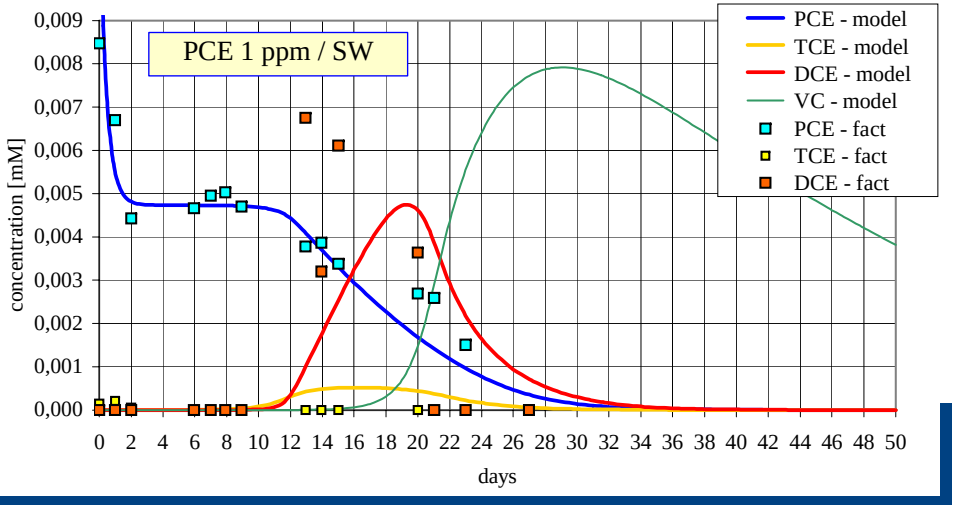
Autoclaved Sediment

	groundwater	surface water
A: 2 000 →	1 →	0.01
B: 100 →	10 →	1
	HW	SW

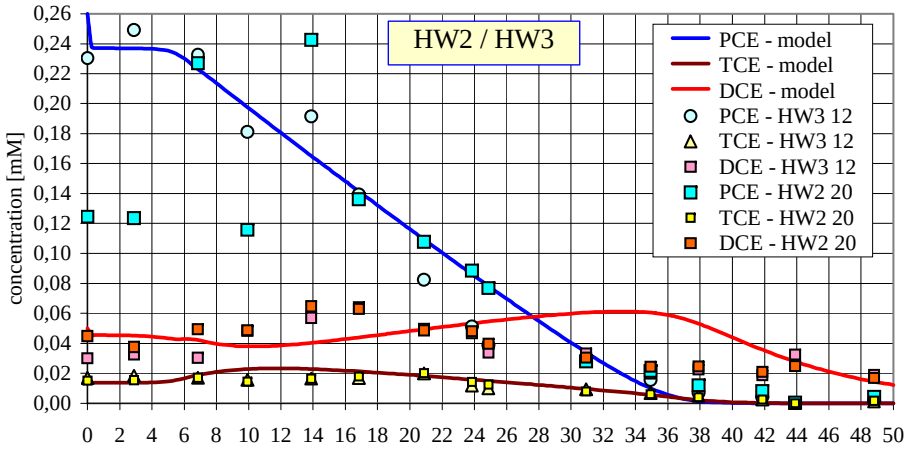
X_0 in µg/L

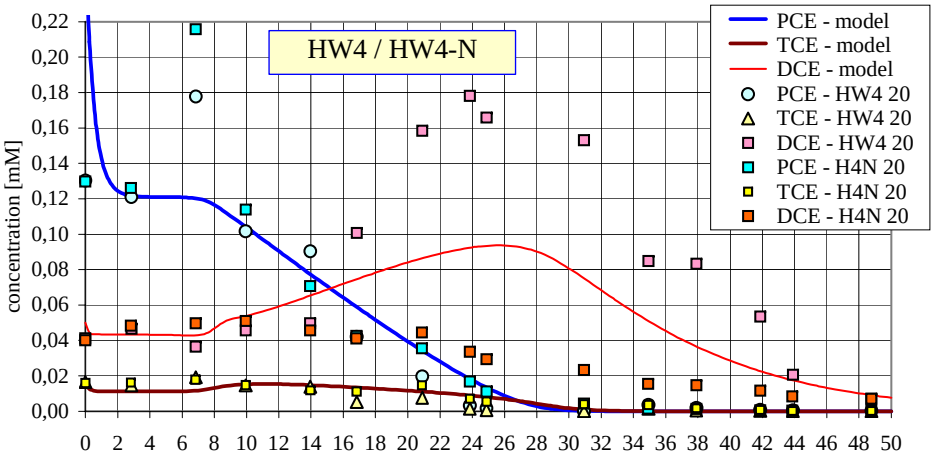


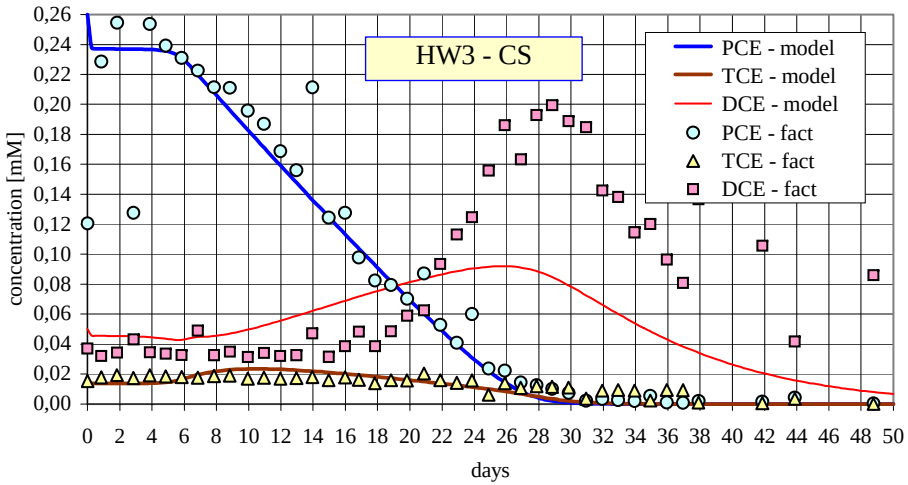


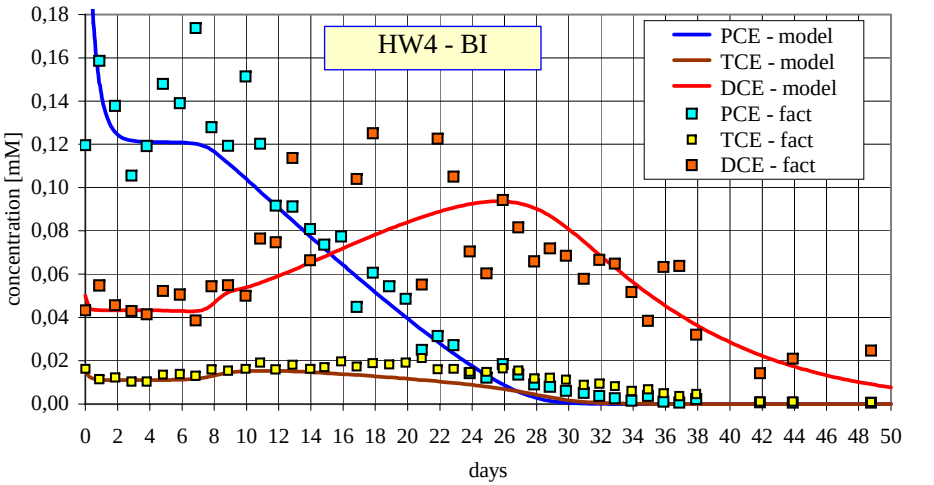


Bela / Aquifer Material

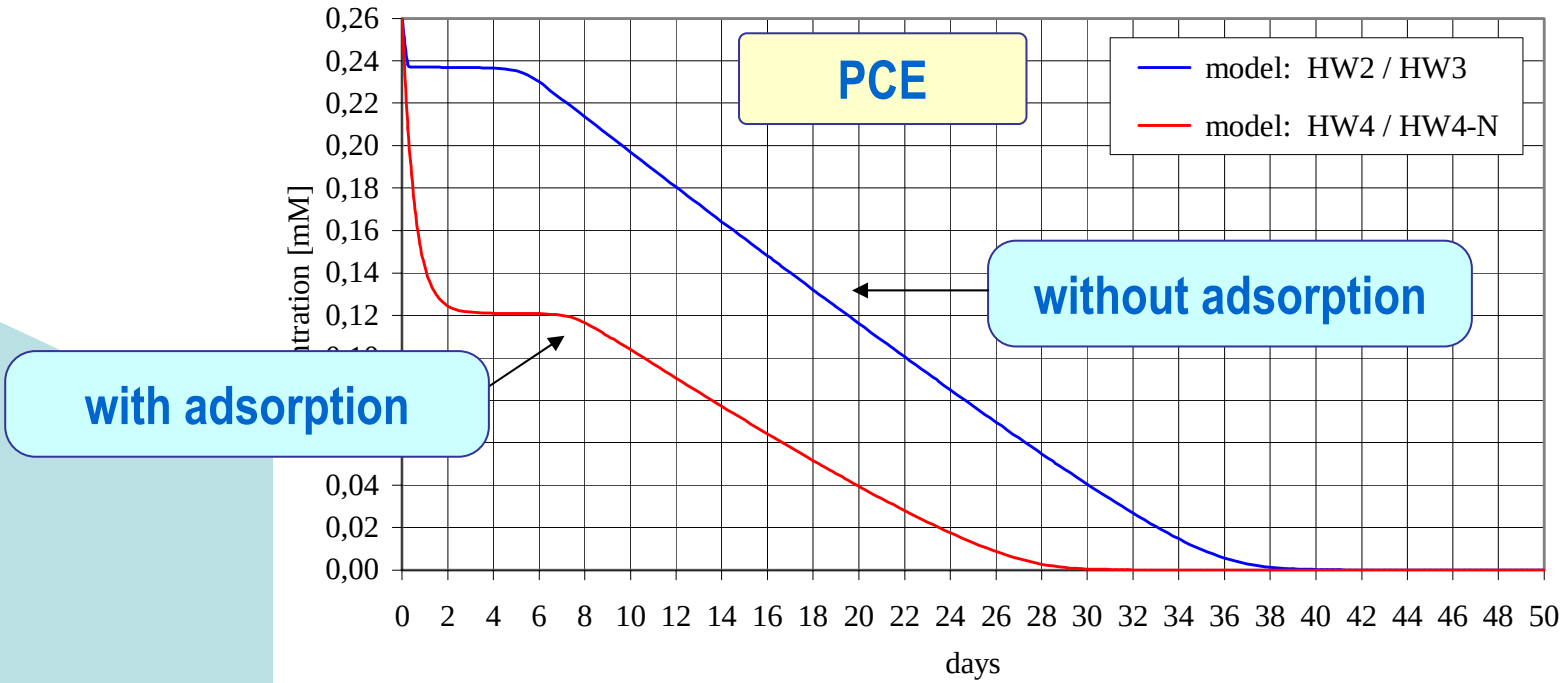








Bela / Aquifer Material



X_0 (aquifer) << X_0 (sediment)

CAH-Modeling

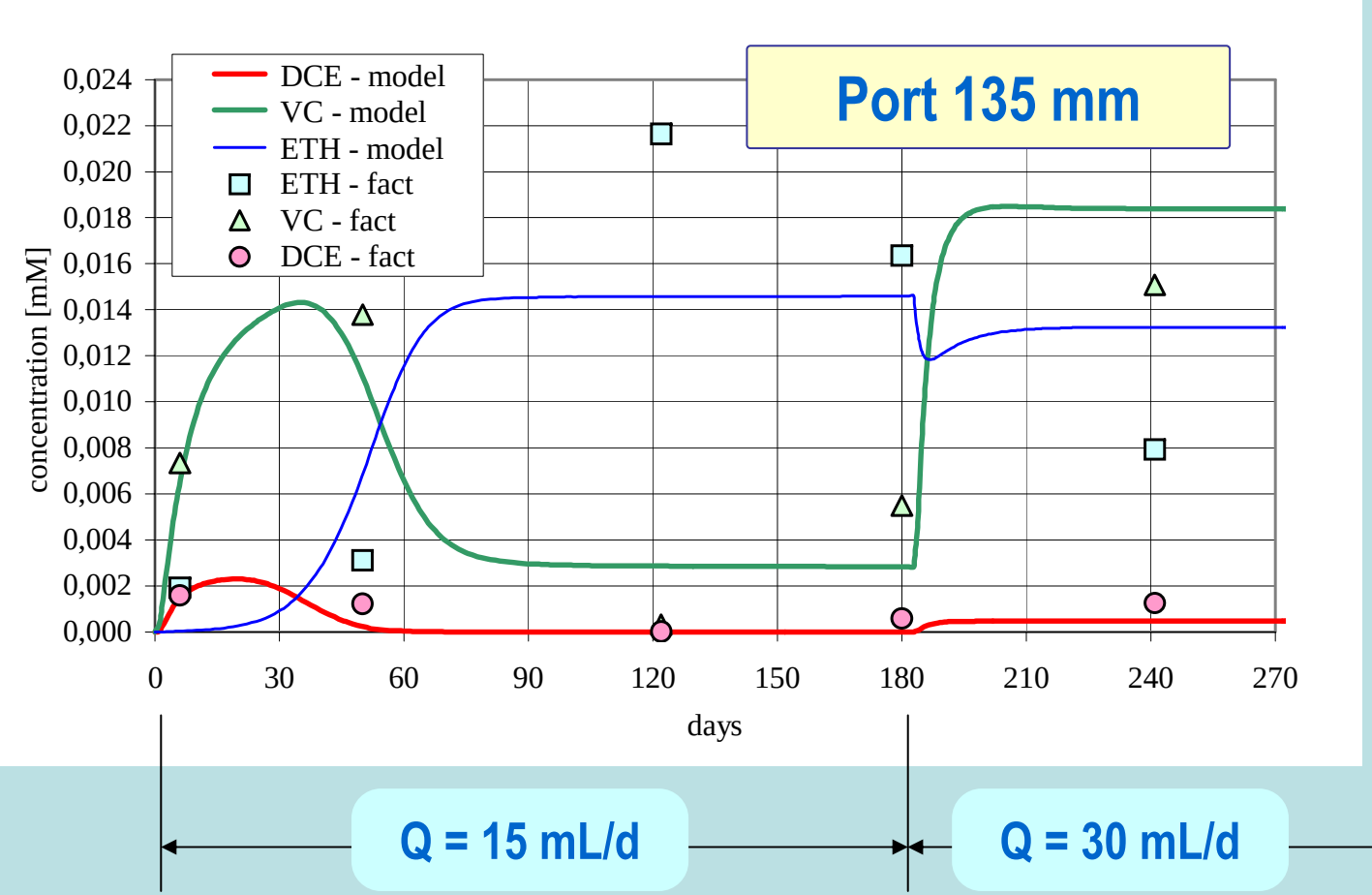
COLUMN TEST

Overview

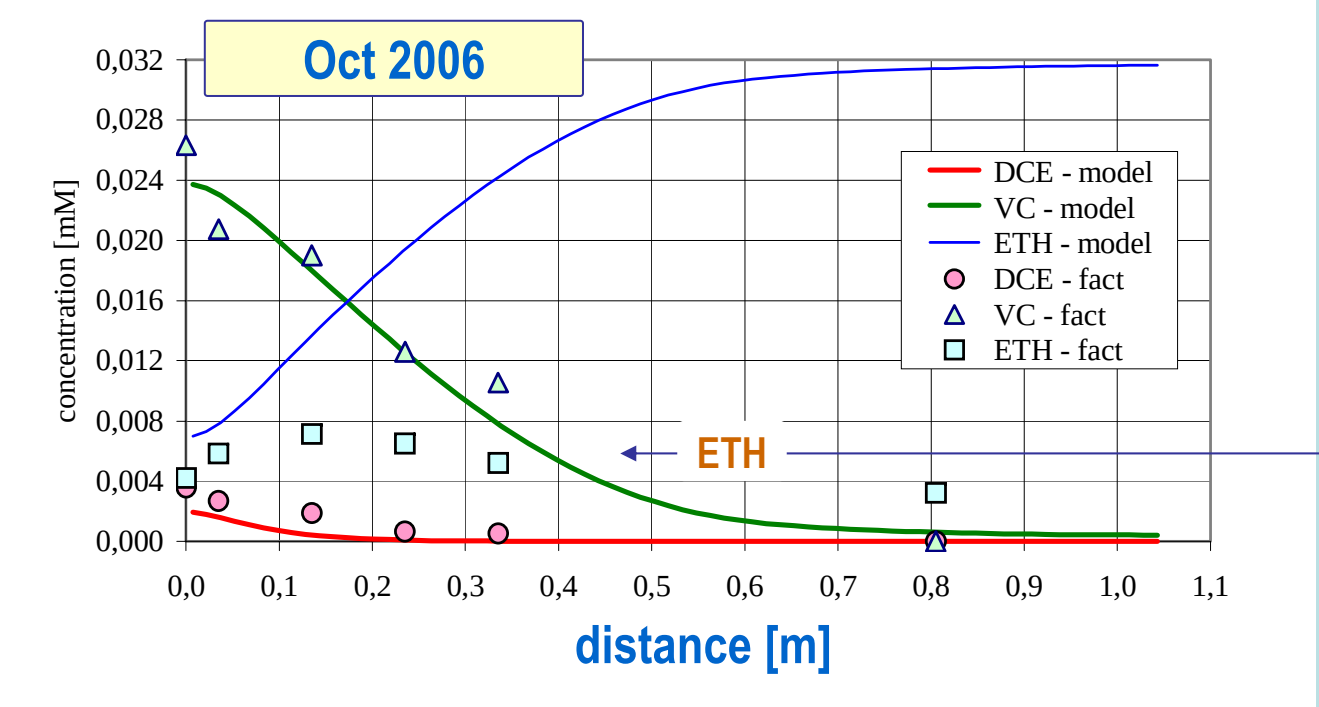
Geometry and Material Parameters

parameter	symbol	unit	Zenne	Bela
column length	L	cm	105	50
cell length	Δx	cm	1.5	2.5
cell number	$N = L/\Delta x$	–	70	20
inner diameter	d	cm	4.2	3.8
cross section	$A = \pi d^2/4$	cm^2	13.85	11.34
porosity	ε	m^3/m^3	0.40	0.31
cell volume	ΔV	cm^3	20.8	28.4
pore volume	$\Delta V_{pore} = \varepsilon \Delta V$	cm^3	8.3	8.8
flow rate	Q	mL/d	15	226
time step (advect.)	$\Delta t = \Delta V_{pore}/Q$	h	13.3	0.93
time step (kinetic)	Δt_{kin}	h	0.83	0.09
sediment density	ρ_{dry}	g/cm^3	1.62	1.23
dispersivity	α	cm	7.5	7.5
org. matter content	f_{OC}	g/g	0.007	0.013

Zenne / Sediment Columns



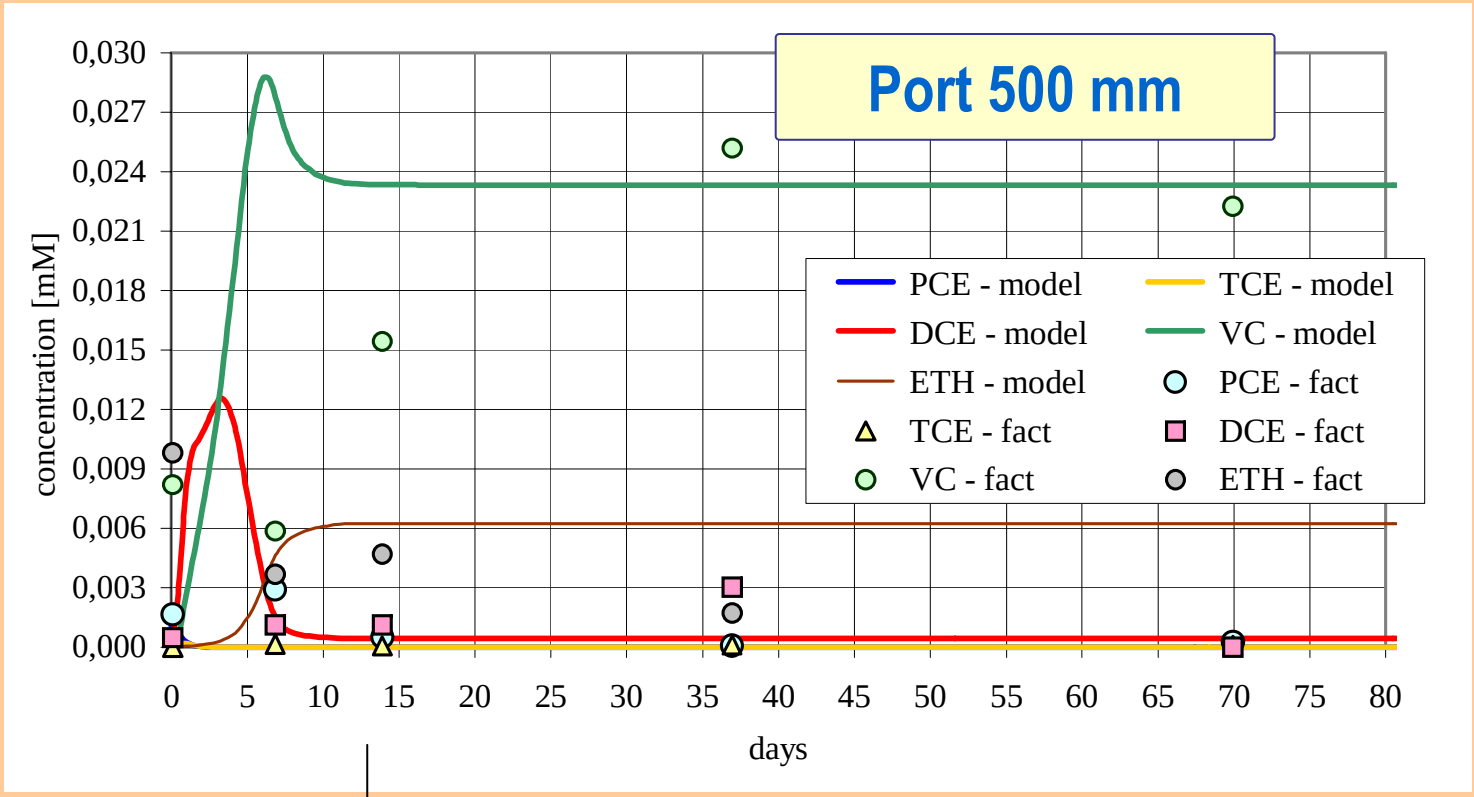
Zenne / Sediment Columns



mass balance ?

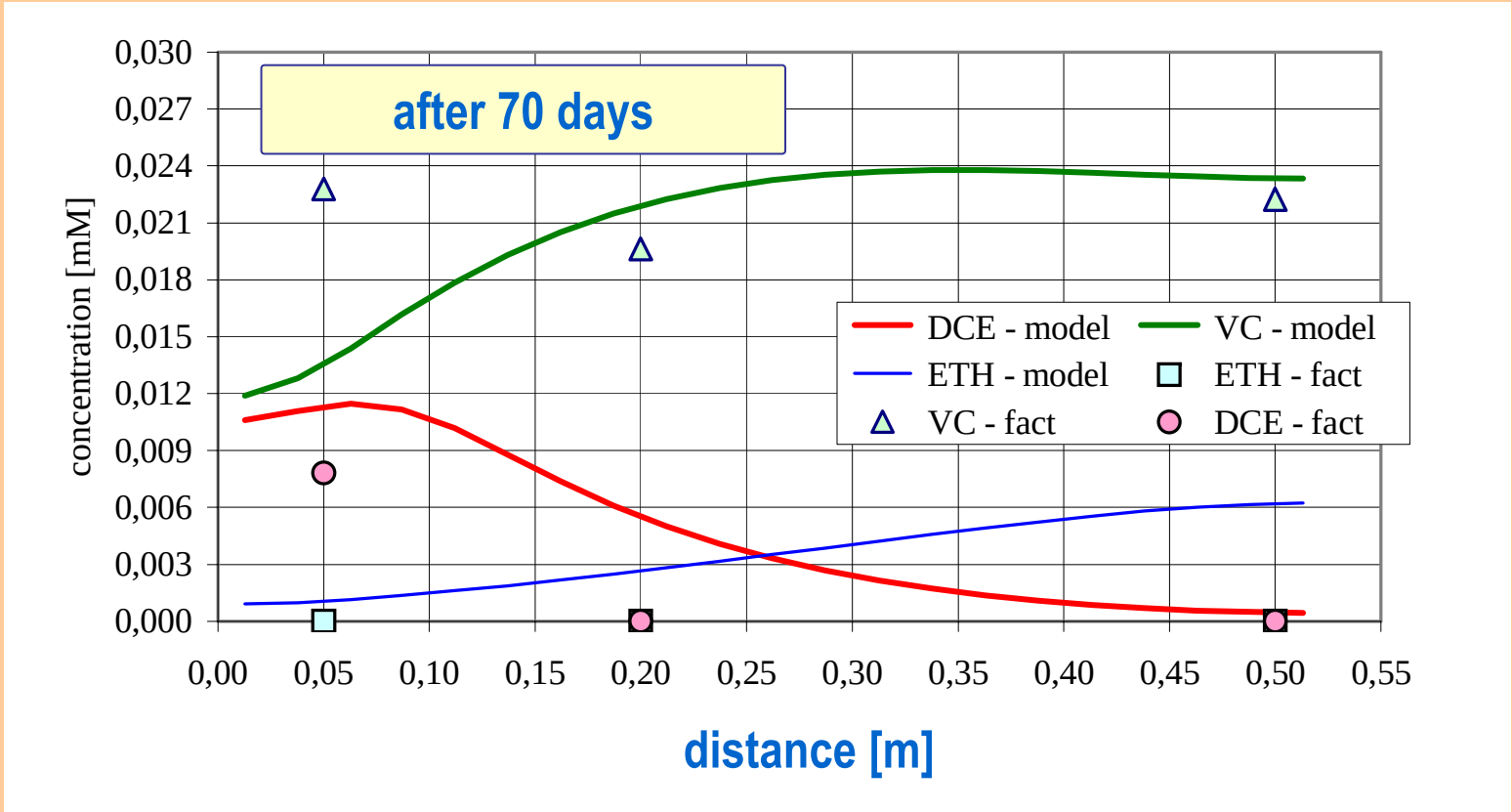
Profile

Bela / Sediment Columns



steady state

Bela / Sediment Columns



Profile

Two-Strain Model

Population Dynamics

$$\frac{dX^{(A)}}{dt} = Y\Omega_A - \Gamma X^{(A)}$$

$$\frac{dX^{(B)}}{dt} = Y\Omega_B - \Gamma X^{(B)}$$

batch	Y = 18 µg/µM
columns	Y = 10 µg/µM

Γ = 0.005 day^{-1}

CAH-Modeling

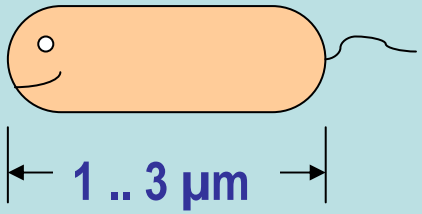
CALCULATING CFU's

Number of Cells per gram dry Soil [cfu/g]

$$n_{cell} = \frac{1}{m_{cell}} \cdot \frac{\varepsilon}{\rho_{dry}} \cdot X$$

biomass per Liter pore water [µg/L]

Bacteria cell



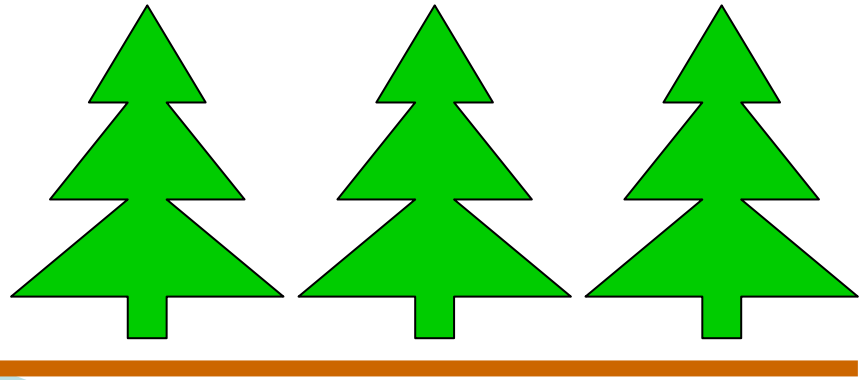
$$m_{cell} = 1.2\,g/cm^3 \cdot 2.5\,\mu m^3 = 3 \cdot 10^{-6}\,\mu g$$

Microbial Diversity

Model

X = 0.01 µg/L	1 cfu / g
X = 6 000 µg/L	$5 \cdot 10^5$ cfu / g

1 strain



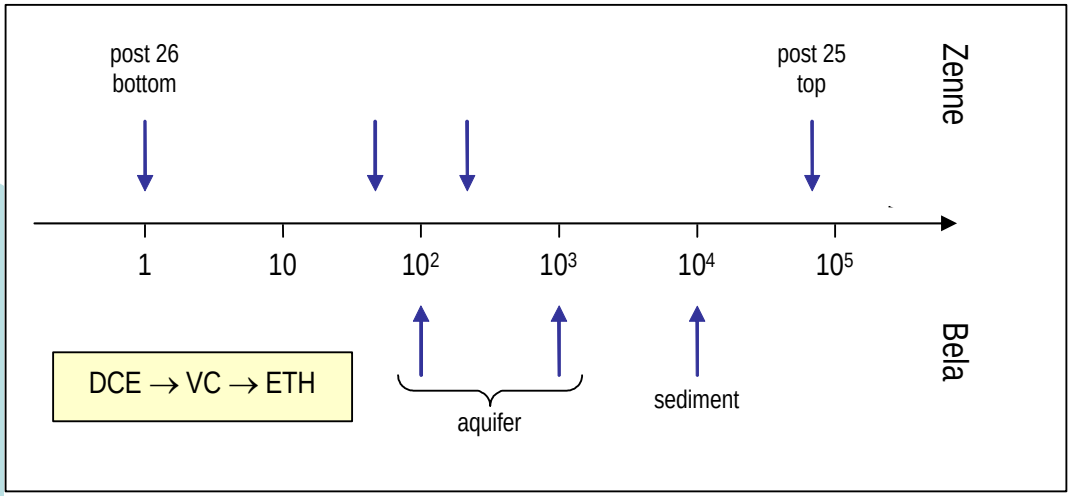
subsurface

10 000 species

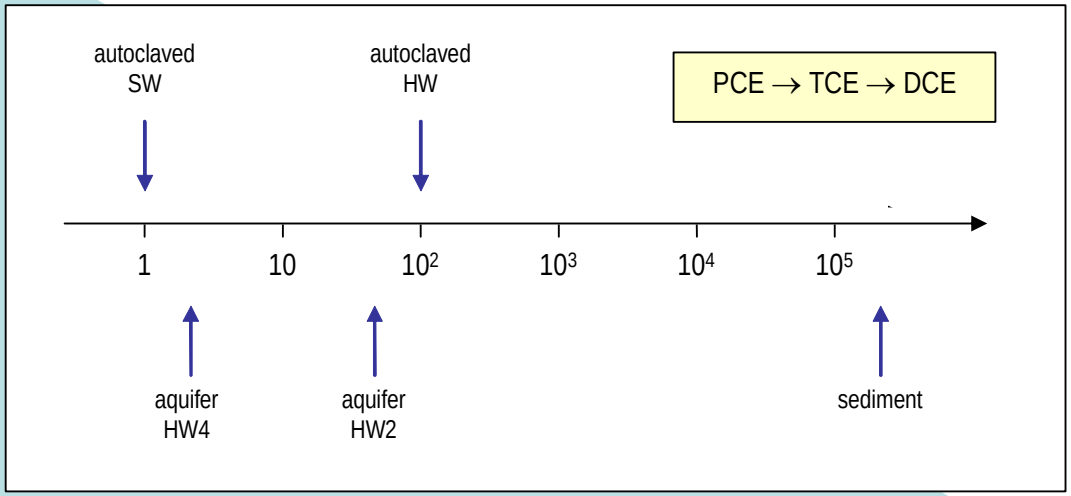
culturable: 10^6 ... 10^8 cells/g

(total: 10^{10} cells/g)

Model Results: CFU/g



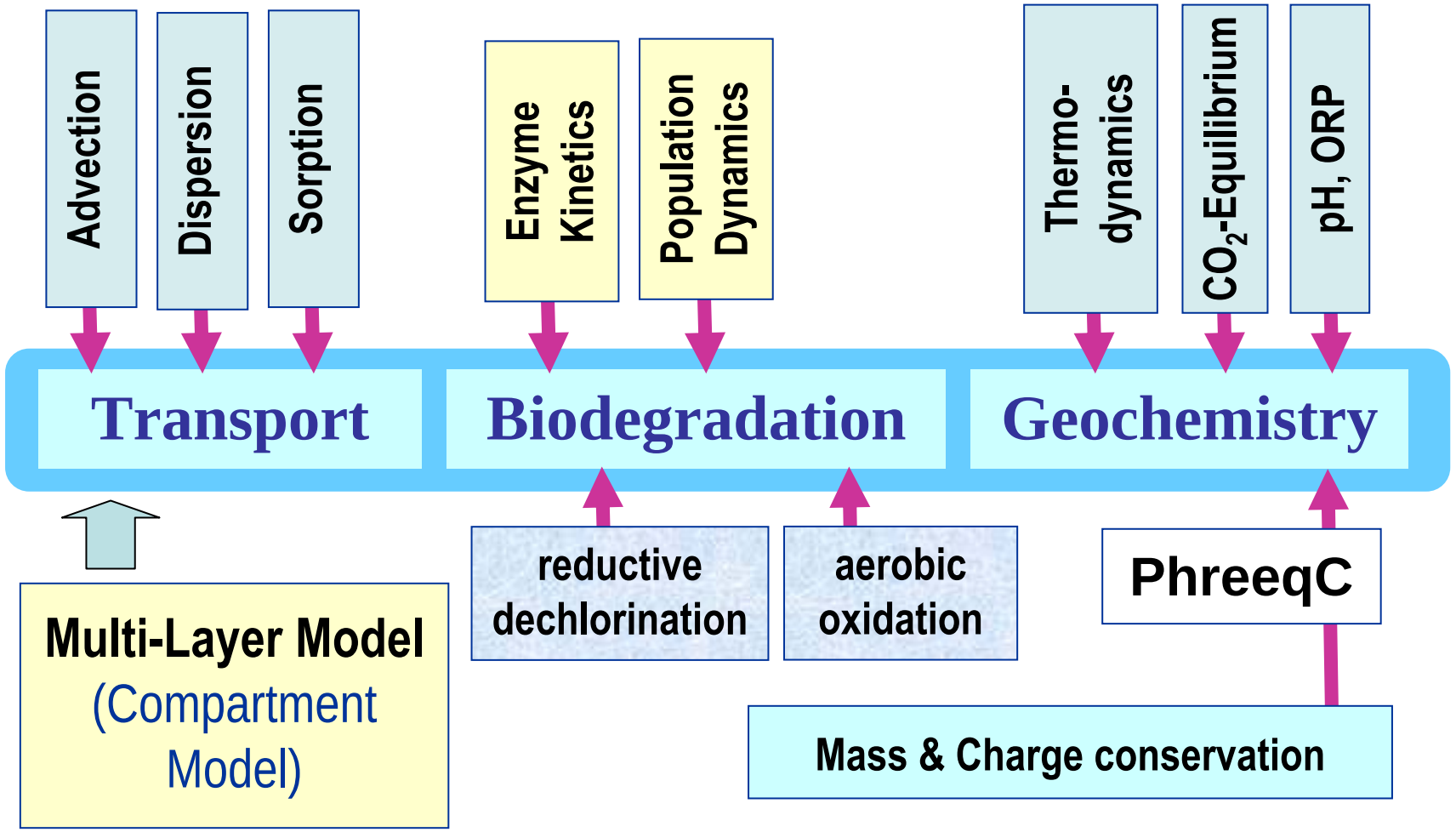
initial population



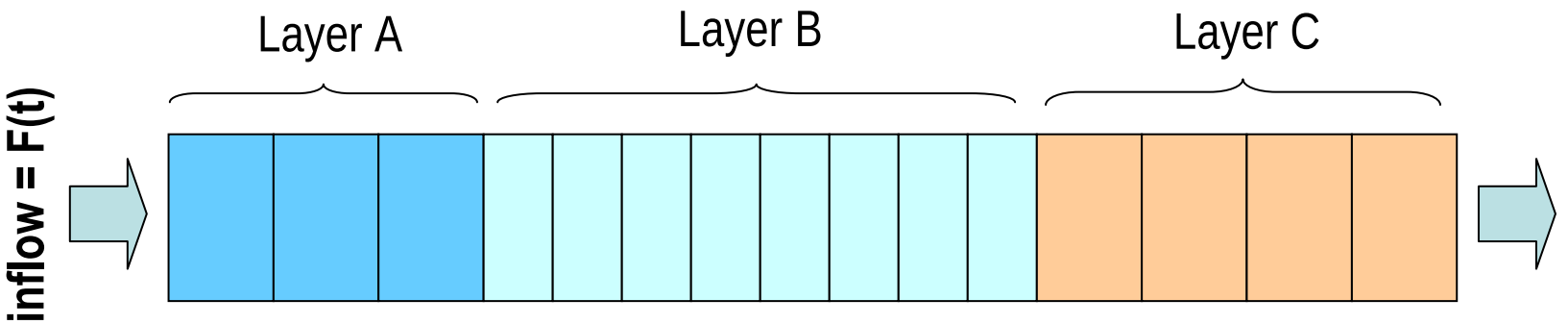
CAH-Modeling

PROGRAM CAPABILITIES

“Between-the-Discipline Model”

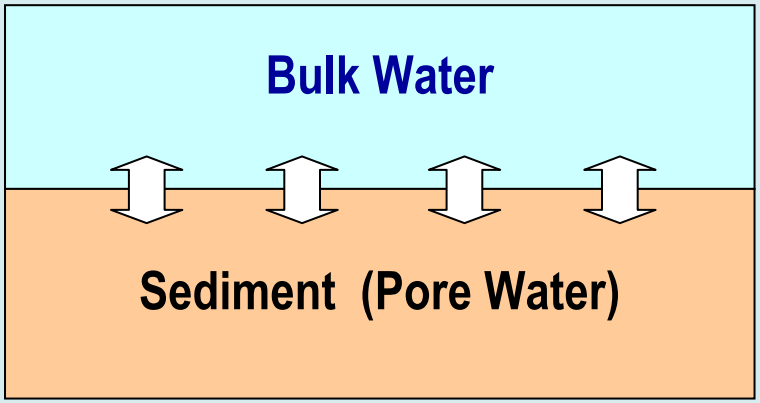


Two Options of the CAH-Model



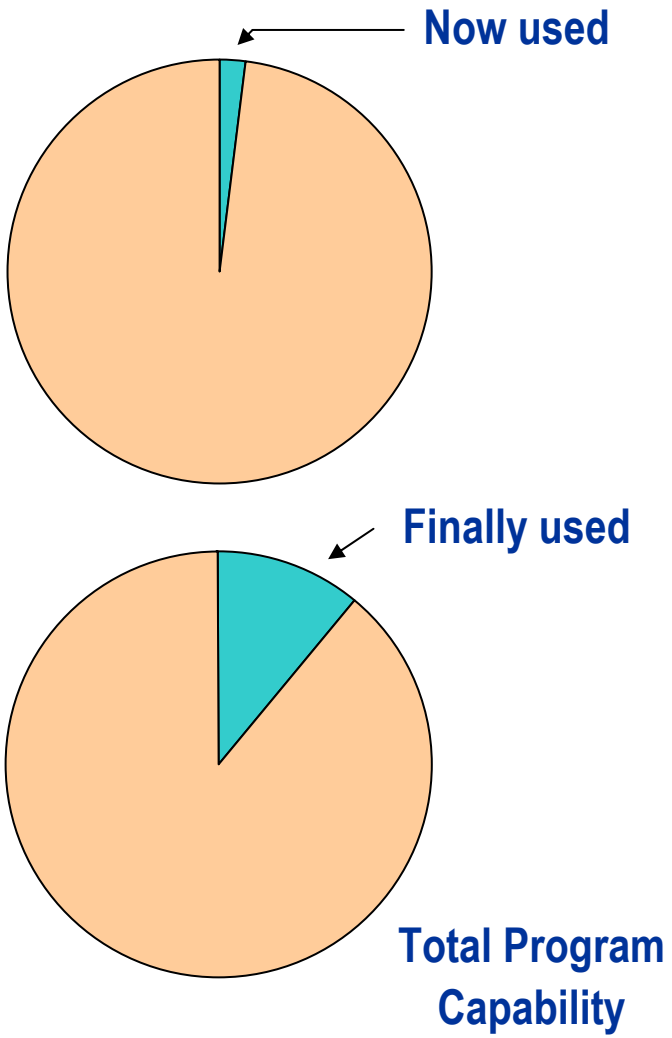
Reactive 1D-Transport

Batch Test
(Kinetics only)



Dynamical-Model Capabilities

		D12	D13
Enzyme Kinetics	Population Dynamics		X
	Anaerobic Pathway	X	X
	Aerobic Pathway		
	T-Dependence		
	pH-Dependence		
	Nutrient Limitation		
	O2-competition		
Transport	Advection + Dispersion		X
	Time-Dependent Inflow		
	Multi-Layer		
	Heterogeneous Populations		
PHREEQC	Complete Analyses		
	Open CO2-System		
	Phase Equilibrium		
	Ion-Exchange		

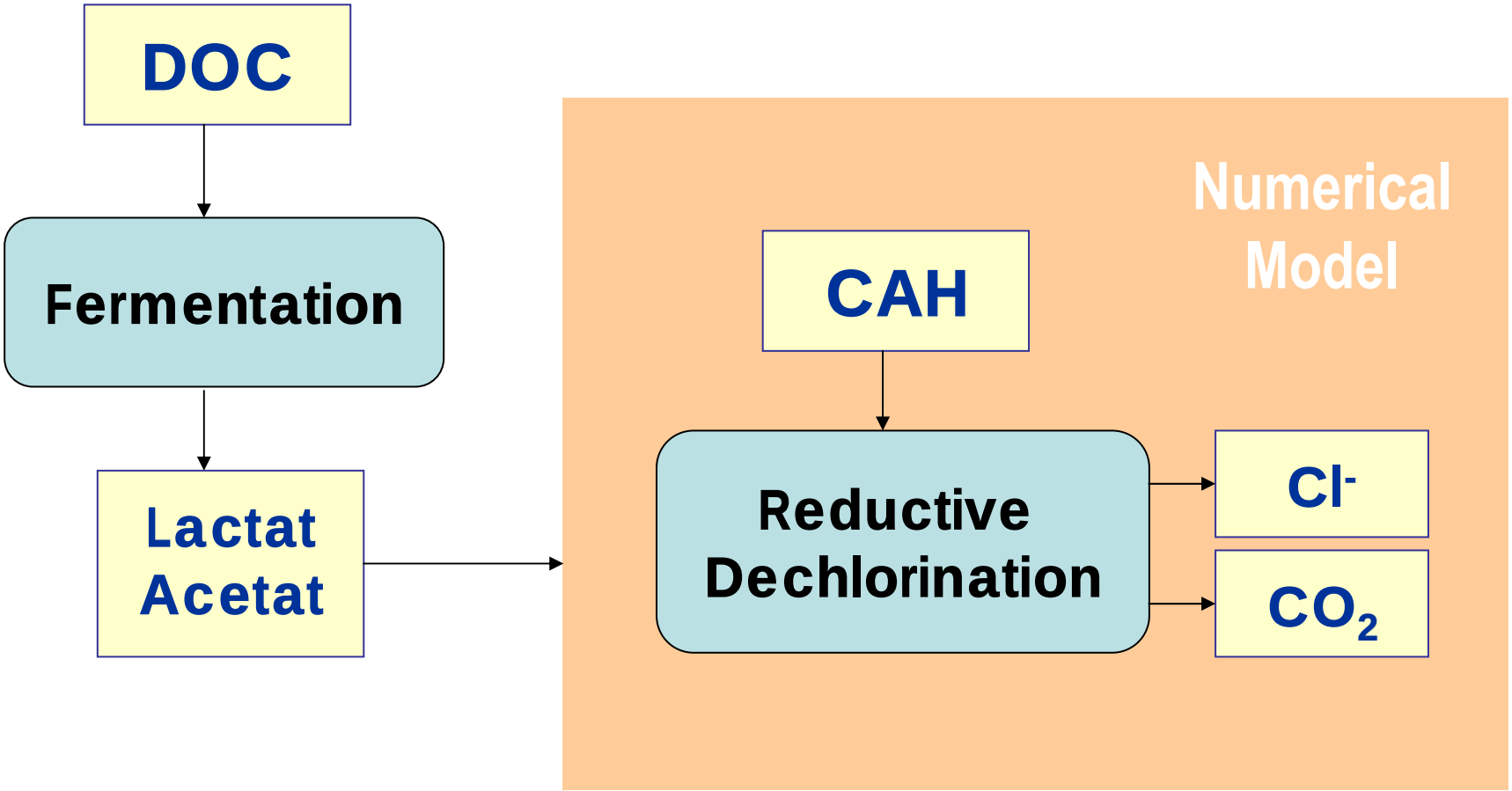


CAH-Modeling

MODEL LIMITATION

Upper Bound for X

Complete Degradation Chain (Symbiosis)



Problem Solving (provisional)

to prevent unlimited population growth →

to simulate limited e-Donor supply →

extra parameter

X_{max}

unaesthetic !

Source Code

```
…
line 5345
line 5346
if ( x > xMAX ) x = xMAX
line 5348
line 5349
…
```

CAH-Modeling

SUMMARY

and Conclusions

Conclusions – Part I

1. "Environmental Microbiology" is highly complex (more than pure culture media)

2. Our approach is only a **first step** towards a "Quanitative Microbiology"

3. **ONE** kinetic dataset exist for batch/column tests from Zenne and Bela sites (but not unique due to unknown X_0)

Batch Reaction Data

	Batch Test	Initial Bulk Water					Initial Pore Water				Adsorption	Sediment			Water	Bacteria Strain A		Bacteria Strain B	
		PCE	TCE	DCE	VC	ETH	PCE	TCE	DCE	VC	f_oc	rho	porosity	m_sed	V_bulk	X_0	X_max	X_0	X_max
		µM	µM	µM	µM	µM	µM	µM	µM	µM	%	g/cm³	m³/m³	g	mL	µg/L	µg/L	µg/L	µg/L
Zenne site	DCE_FAST			3,6	8	1,5			3,6	8	0,7	1,62	0,40	30	70			800	4000
	DCE_MID			3,6	8	1,5			3,6	8	0,7	1,62	0,40	30	70			2	4000
	DCE_SLOW			3,6	8	1,5			3,6	8	0,7	1,62	0,40	30	70			0,5	4000
	DCE_XSLOW			3,6	8	1,5			3,6	8	0,7	1,62	0,40	30	70			0,01	4000
	VC_XFAST				35	10				35	0,7	1,62	0,40	30	70			3000	
	VC_ FAST				35	5				35	0,7	1,62	0,40	30	70			2400	6000
	VC_MID				35	5				35	0,7	1,62	0,40	30	70			1400	5000
	VC_LOW				35	5				35	0,7	1,62	0,40	30	70			700	3500
Bela site	DCE_1			10,3					5		1,3	1,23	0,31	58	110			100	1400
	DCE_10			103,2					5		1,3	1,23	0,31	58	110			100	1400
	DCE_50			300					5		1,3	1,23	0,31	58	110			100	1400
	PCE_1	6					3				1,3	1,23	0,31	58	110	2000	6000	100	1400
	PCE_10	60,3					3				1,3	1,23	0,31	58	110	2000	6000	100	1400
	PCE_50	220									1,3	1,23	0,31	58	110	2000	6000	100	1400
	DCE_HW			103							0,4	1,23	0,31	58	110			10	1400
	DCE_SW			103							0,4	1,23	0,31	58	110			1	500
	PCE_HW	12									0,4	1,23	0,31	58	110	1	500	10	1400
	PCE_SW	12									0,4	1,23	0,31	58	110	0,01	200	1	500
	HW2	260	15	50							0	1,14	0,21	58	110	0,5	1800	10	2800
	HW3_CS	260	15	50							0	1,14	0,21	58	110	0,5	2600	10	2800
	HW4	260	15	50							0,3	1,14	0,21	58	110	0,02	3000	1	2800
	HW4_BI	260	15	50							0,3	1,14	0,21	58	110	0,02	3000	1	2800

Conclusions – Part II

4 Population is time-dependent (non-constant);
at least two strains for complete CAH-degradation

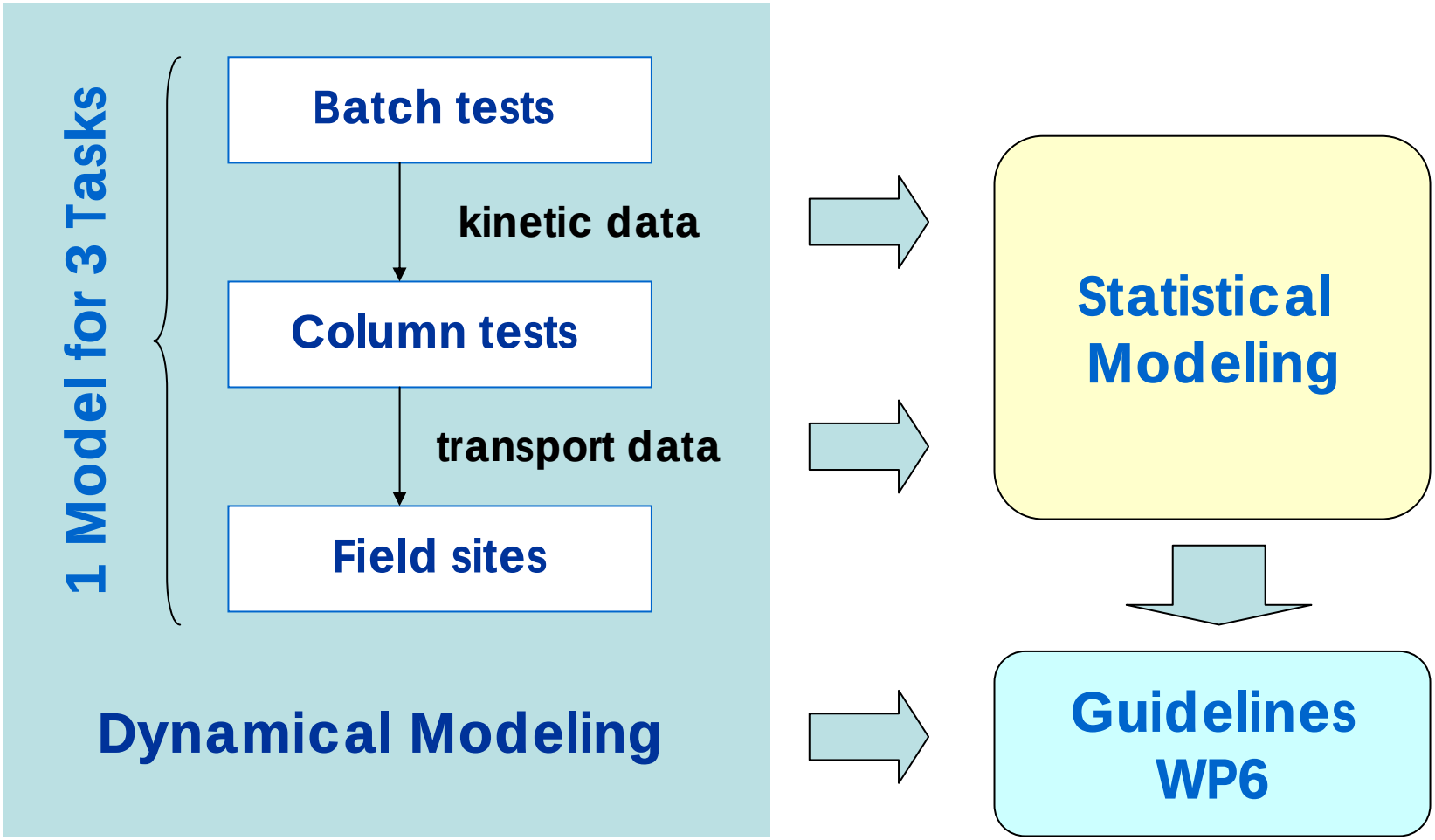
5 Deduced CFU's are in accord with other estimations

OUTLOOK - Future Model Extensions:

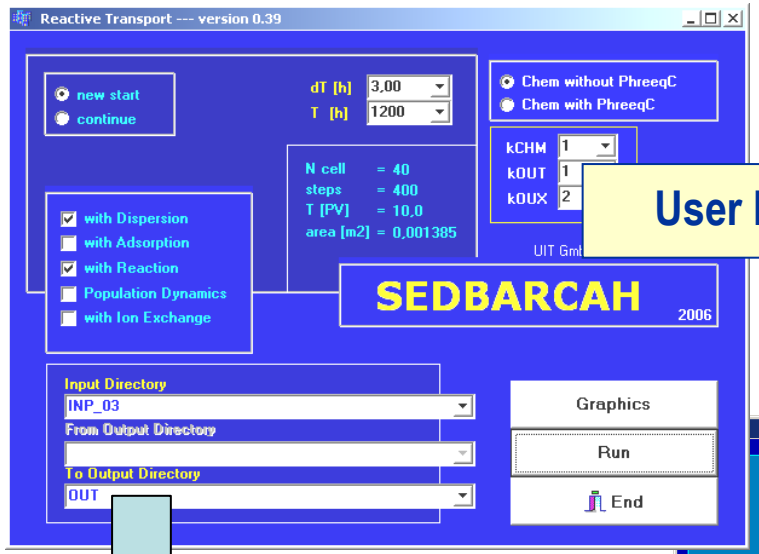
Symbiosis of fermentative and respirative bacteria

Calculation of $\delta^{13}C$ data (for isotopic analysis)

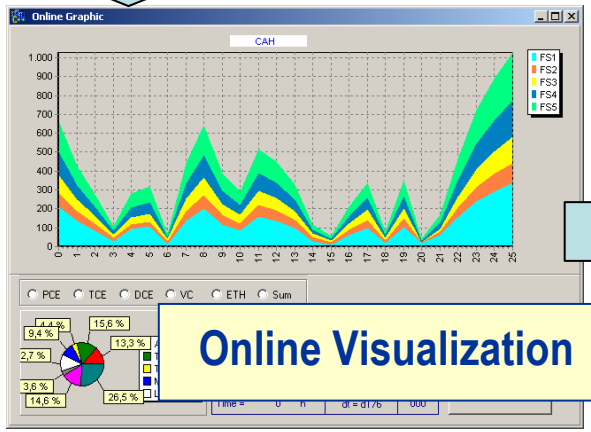
Modeling in WP5



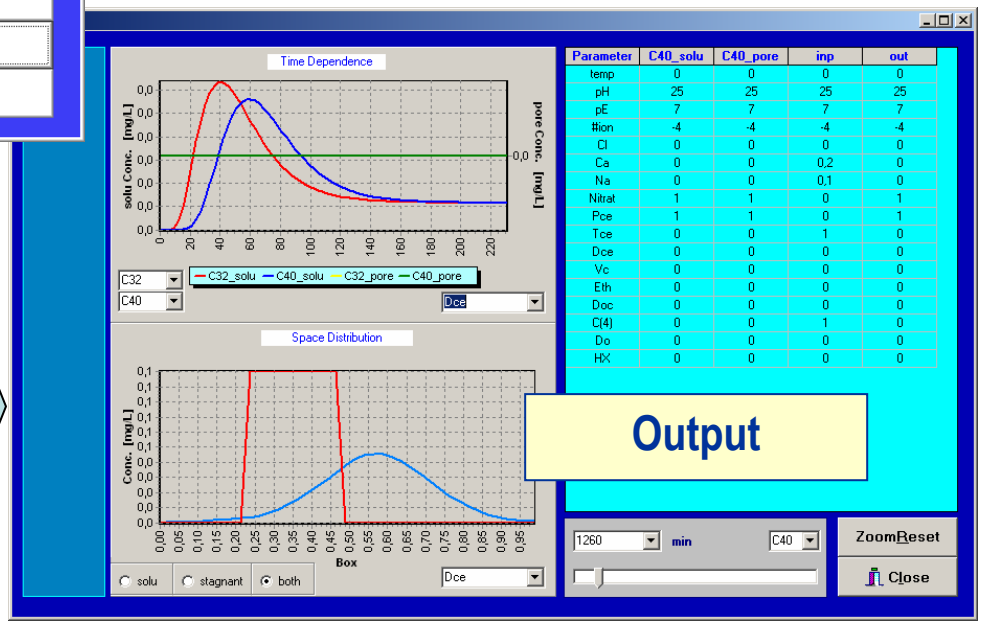
SEDBARCAH Computer Program



User Interface



Online Visualization



Output

- fast C++ code
- incl. PhreeqC
- high flexibility