

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
Lead contractor for Work Package 5 (Modeling):

Duration: 2 years
UIT GmbH Dresden

CAH-Modeling

SEDBARCAH

1 Basic Idea

2 DCE & VC degradation

3 The Complete Chain

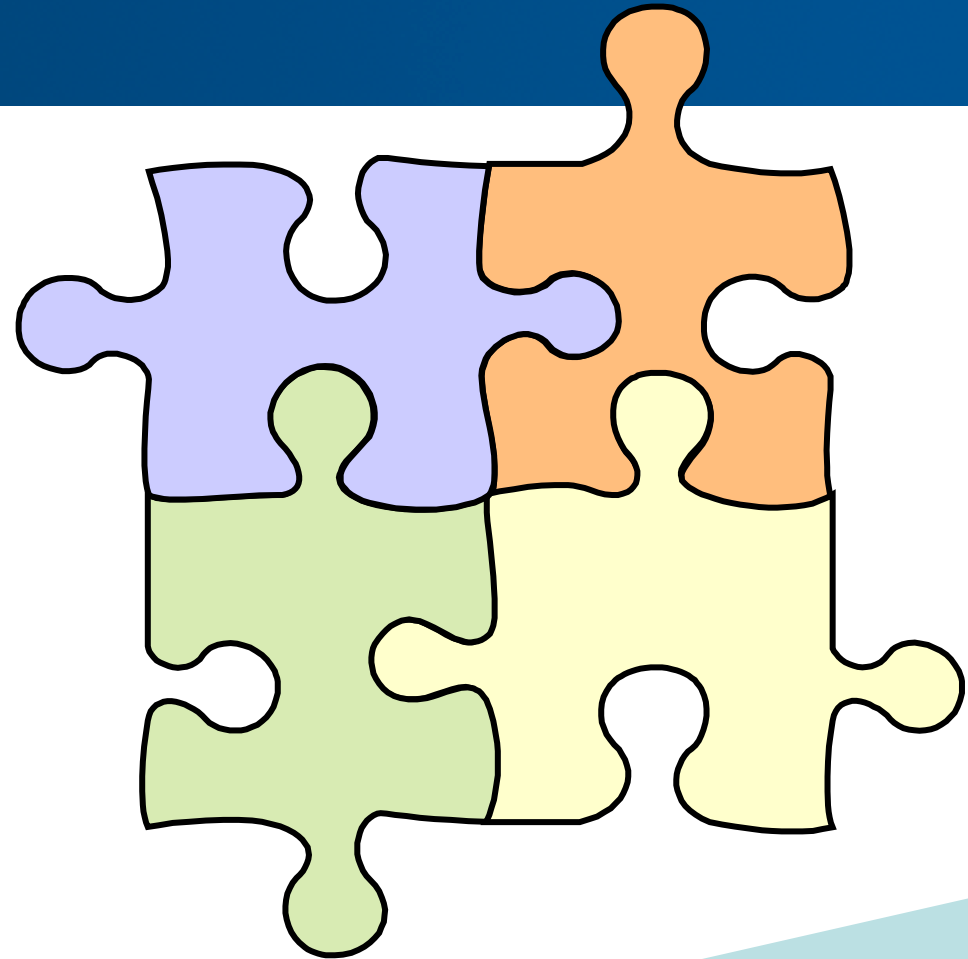
4 Column Tests

5 Conclusions & Outlook

The D13 Puzzle

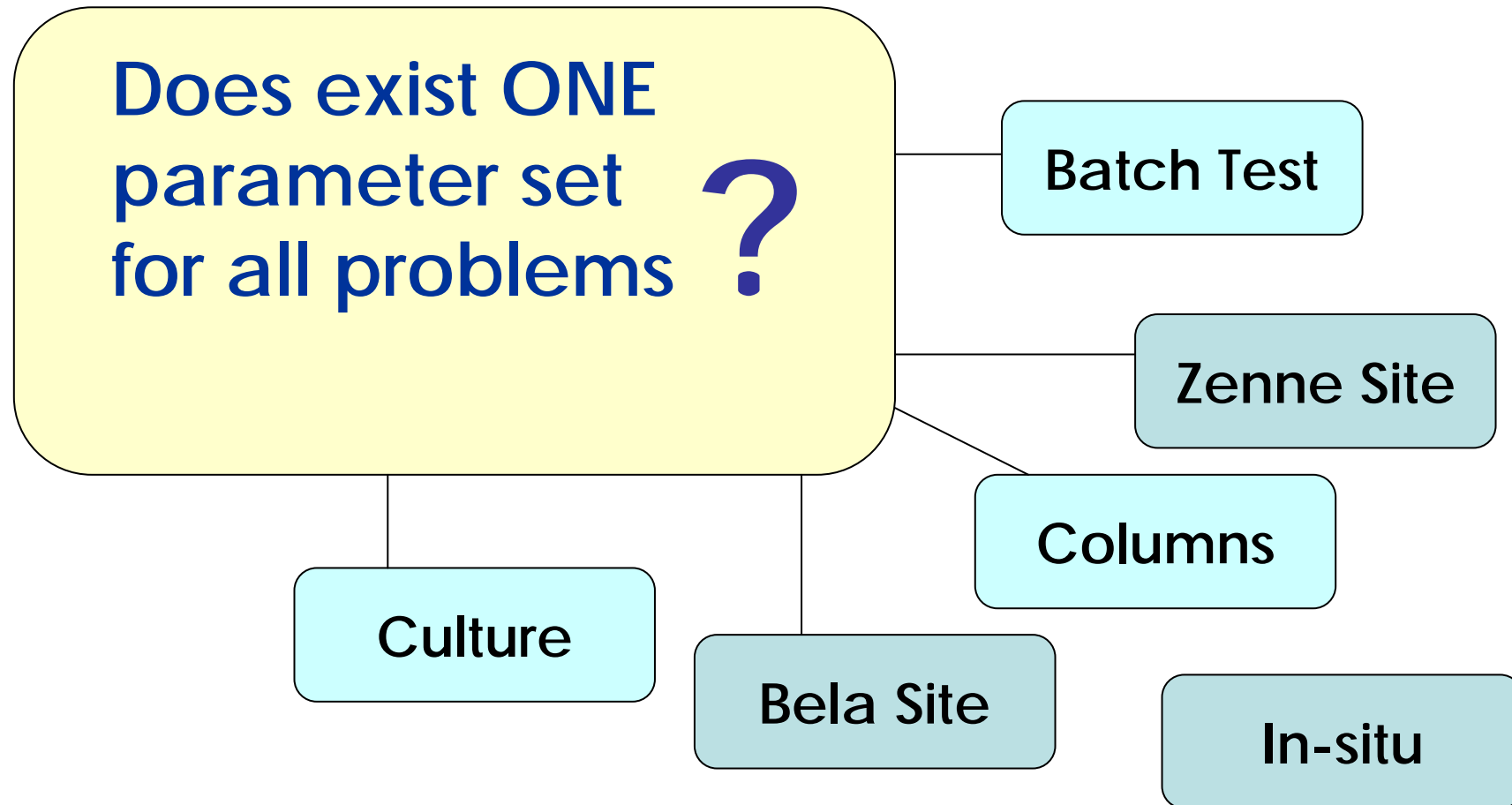
A huge number of experiments.

About 30 model parameters.

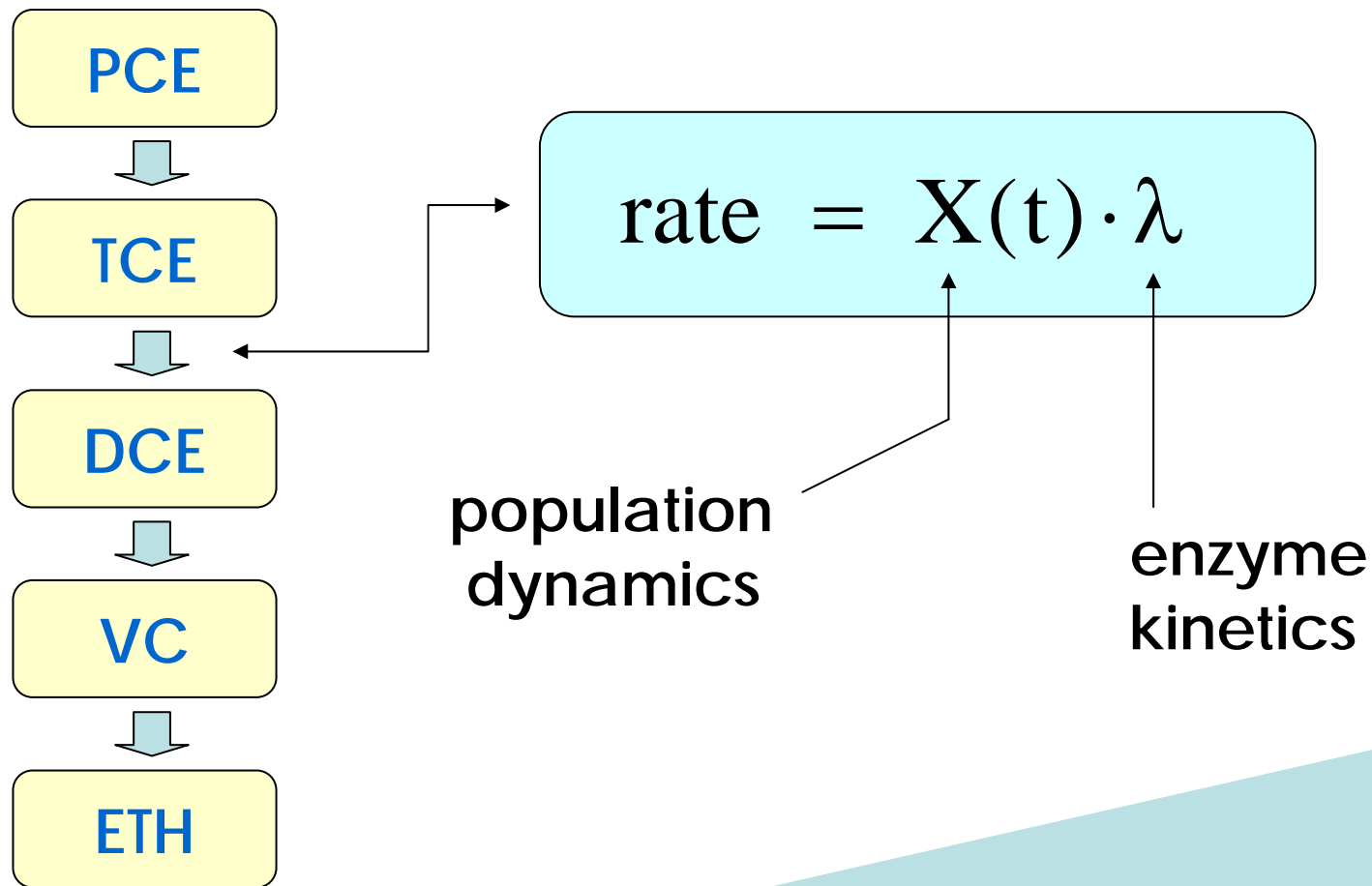


4 000 Calculations

Main Question



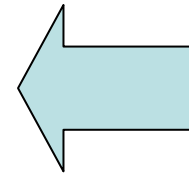
Basic Idea



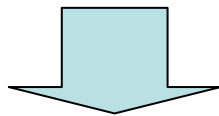
Factorization Ansatz

Kinetic Parameter Set

	k_i	K_i	K_{ii}
	$\mu\text{mol}/\mu\text{g}/\text{d}$	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

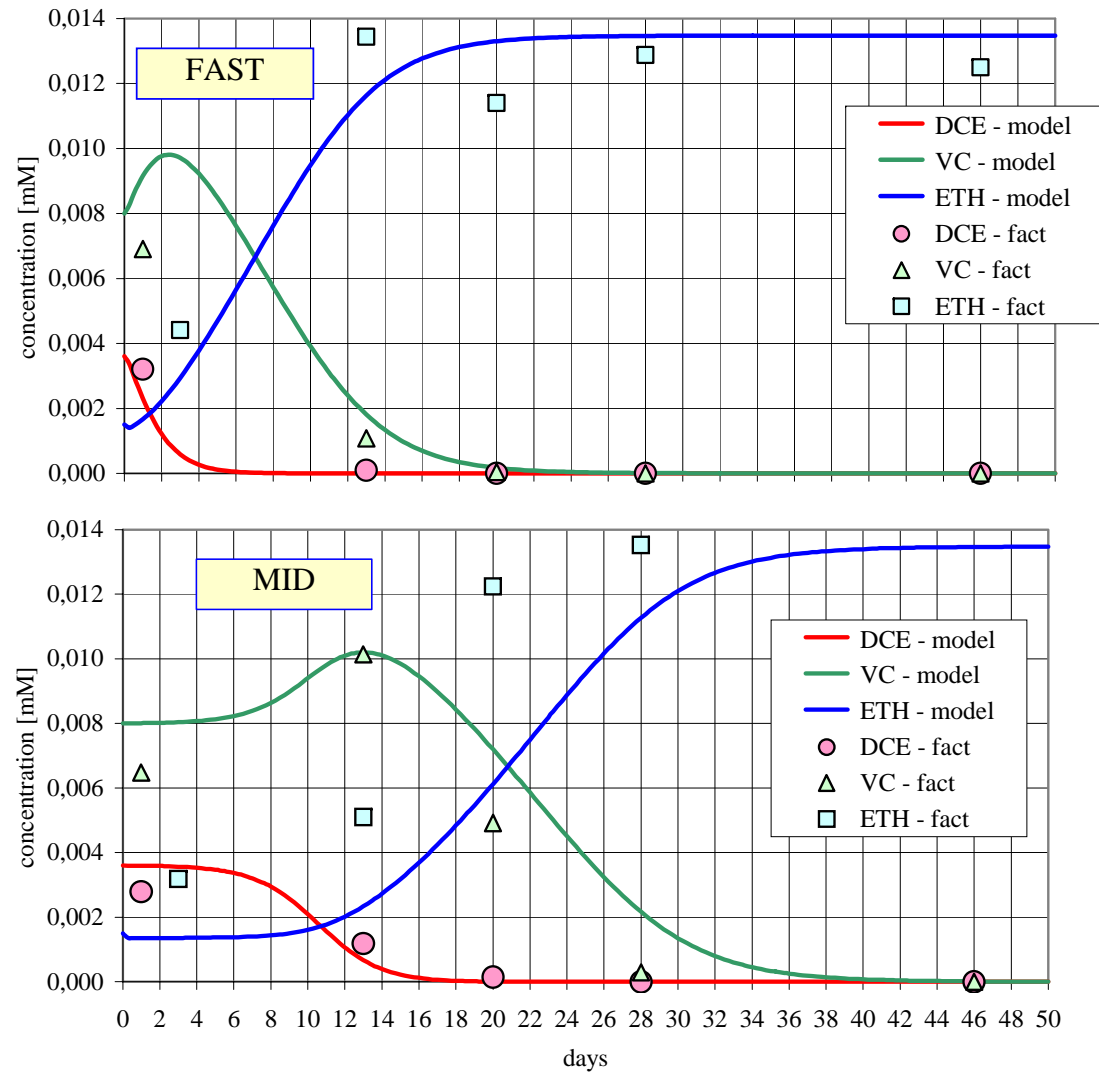
modified literature data

Zenne / DCE degradation

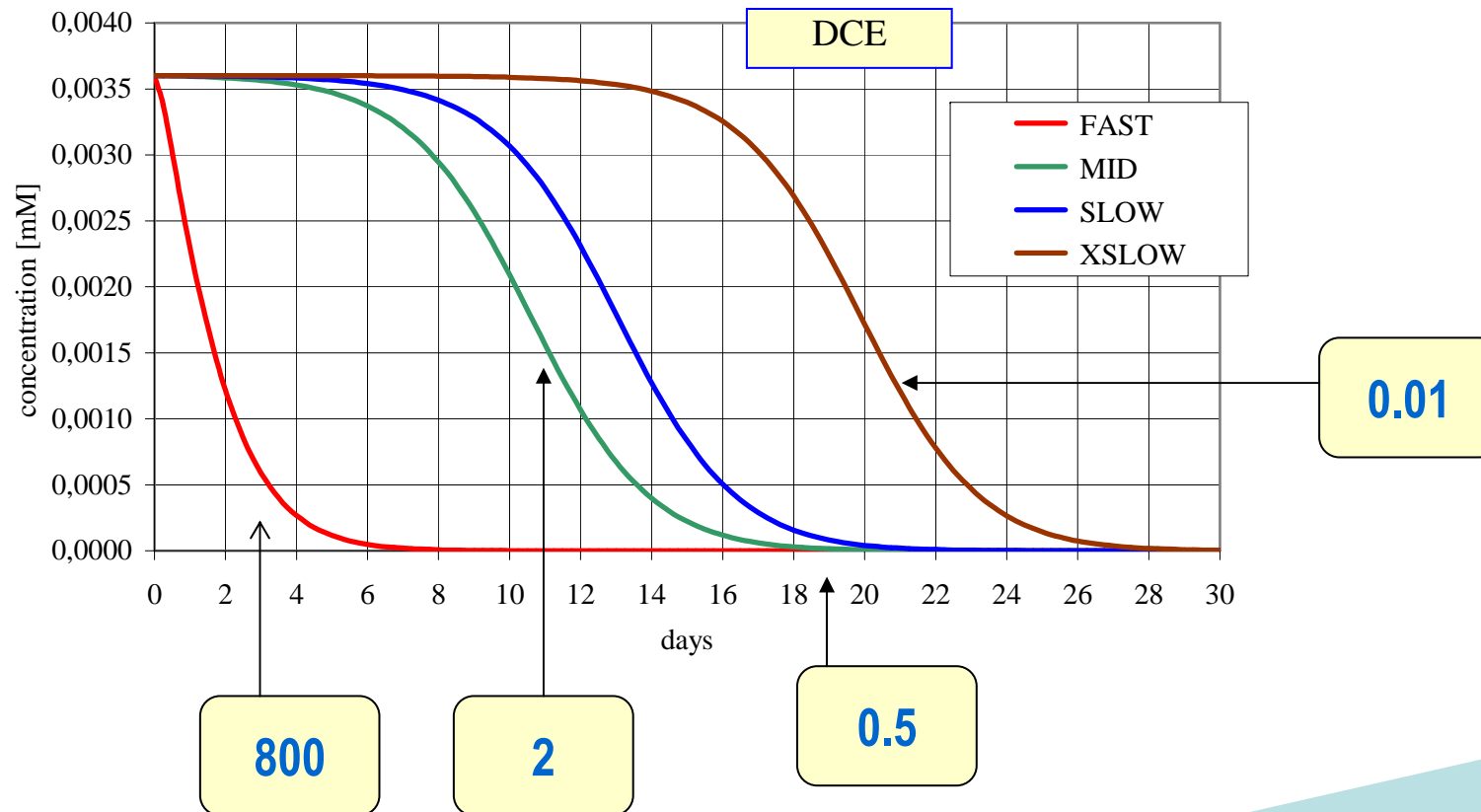
	initial population X_0
	$\mu\text{g/L}$ pore water
FAST	800
MID	2
SLOW	0.5
xSLOW	0.01

all data
bundled into
4 groups

fitted
parameter



Variation of X_0



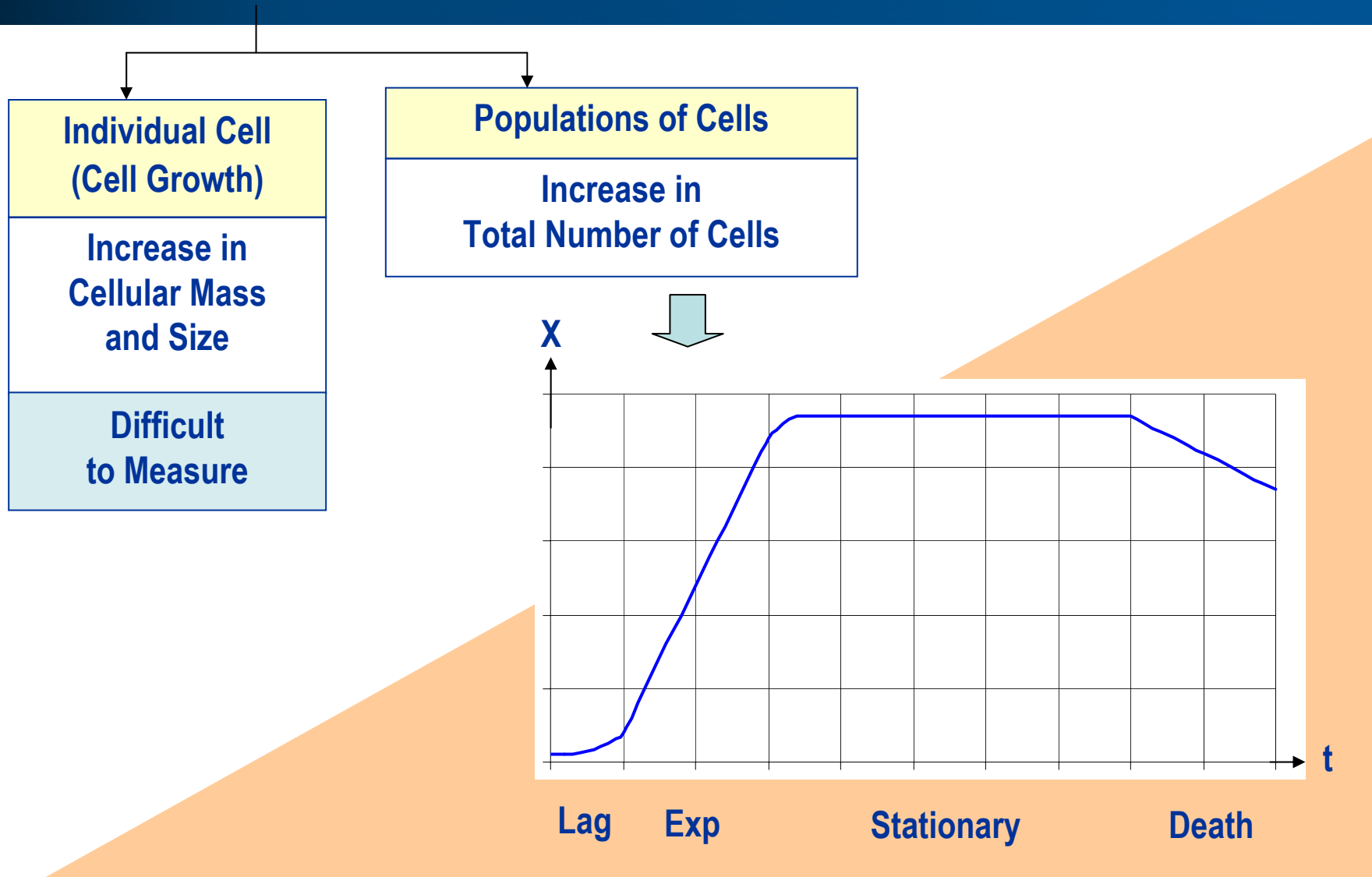
initial biomass in $\mu\text{g/L}$

CAH-Modeling

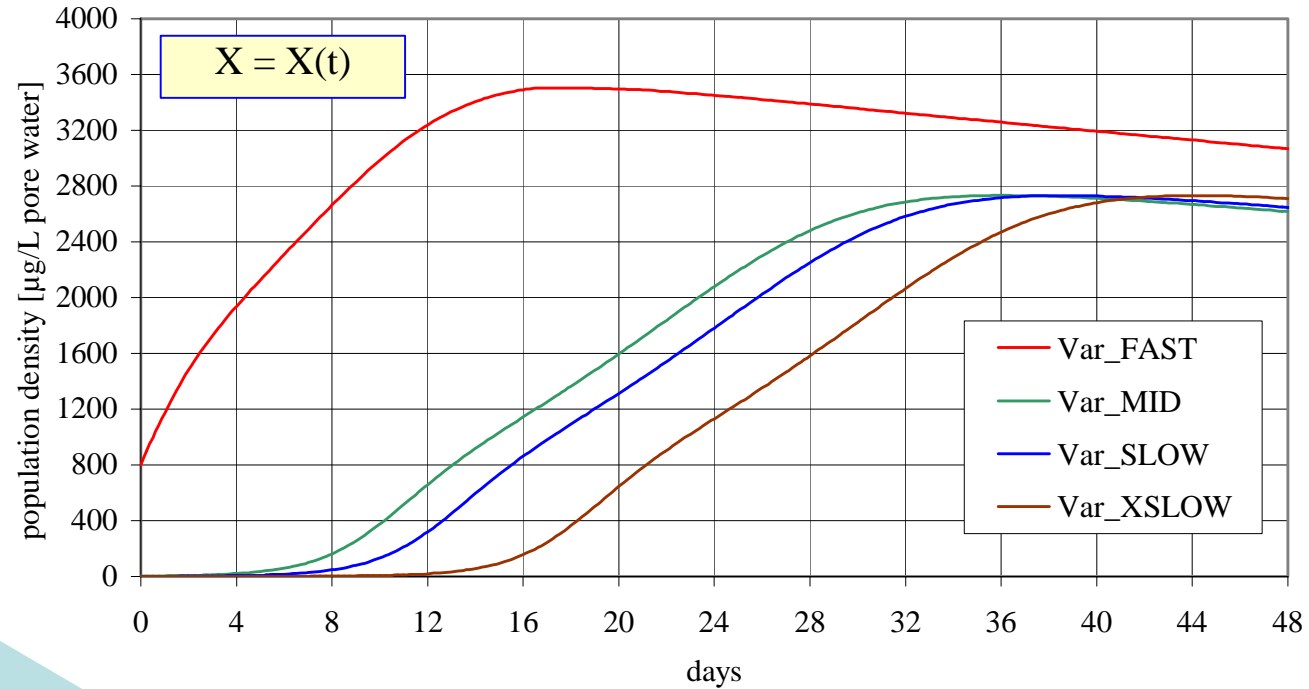
Population
Dynamics

Zenne DCE

Bacterial Growth



Population Growth for various X_0



yield

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

death rate

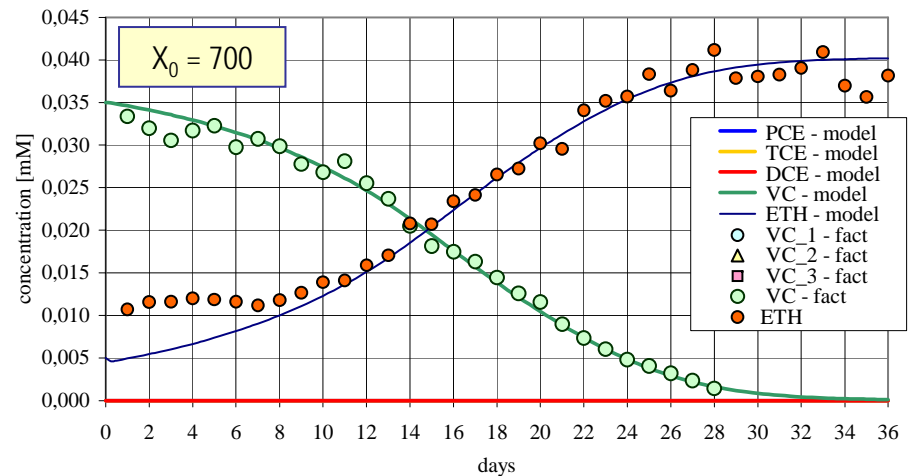
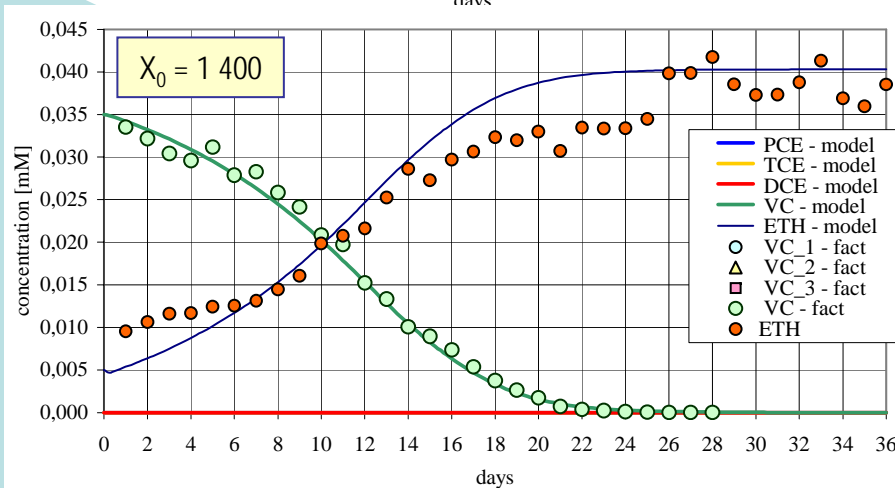
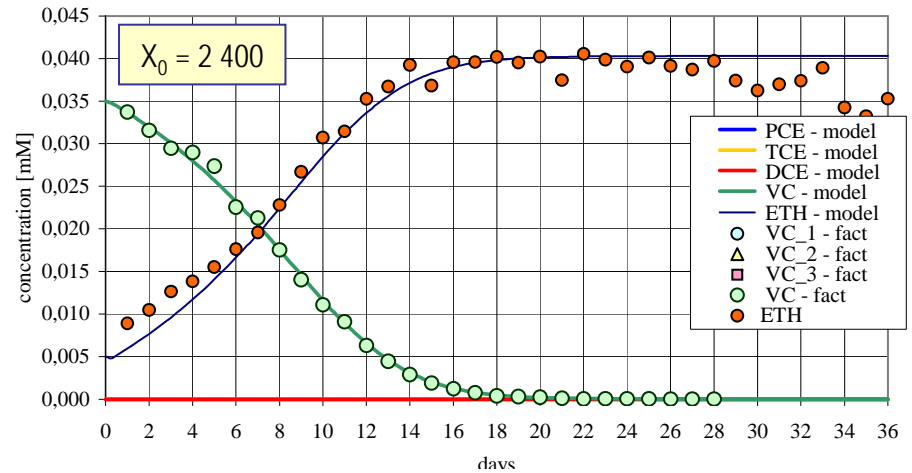
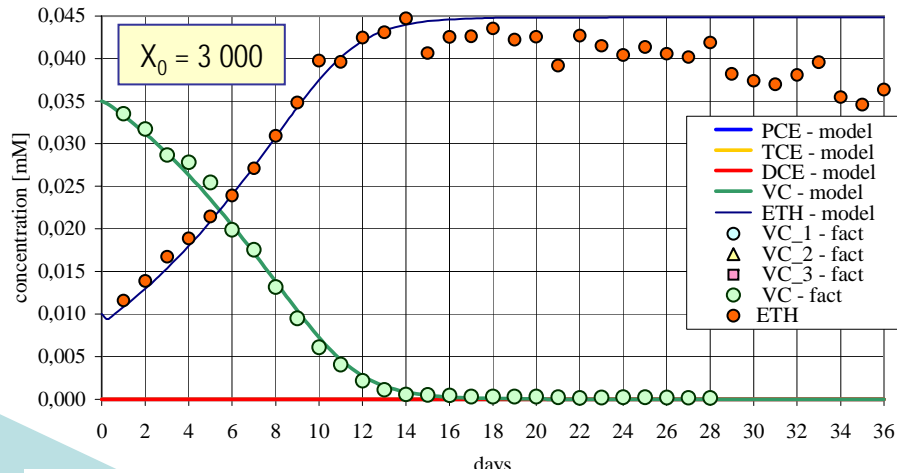
Zenne DCE

CAH-Modeling

BATCH TEST

VC and DCE degradation

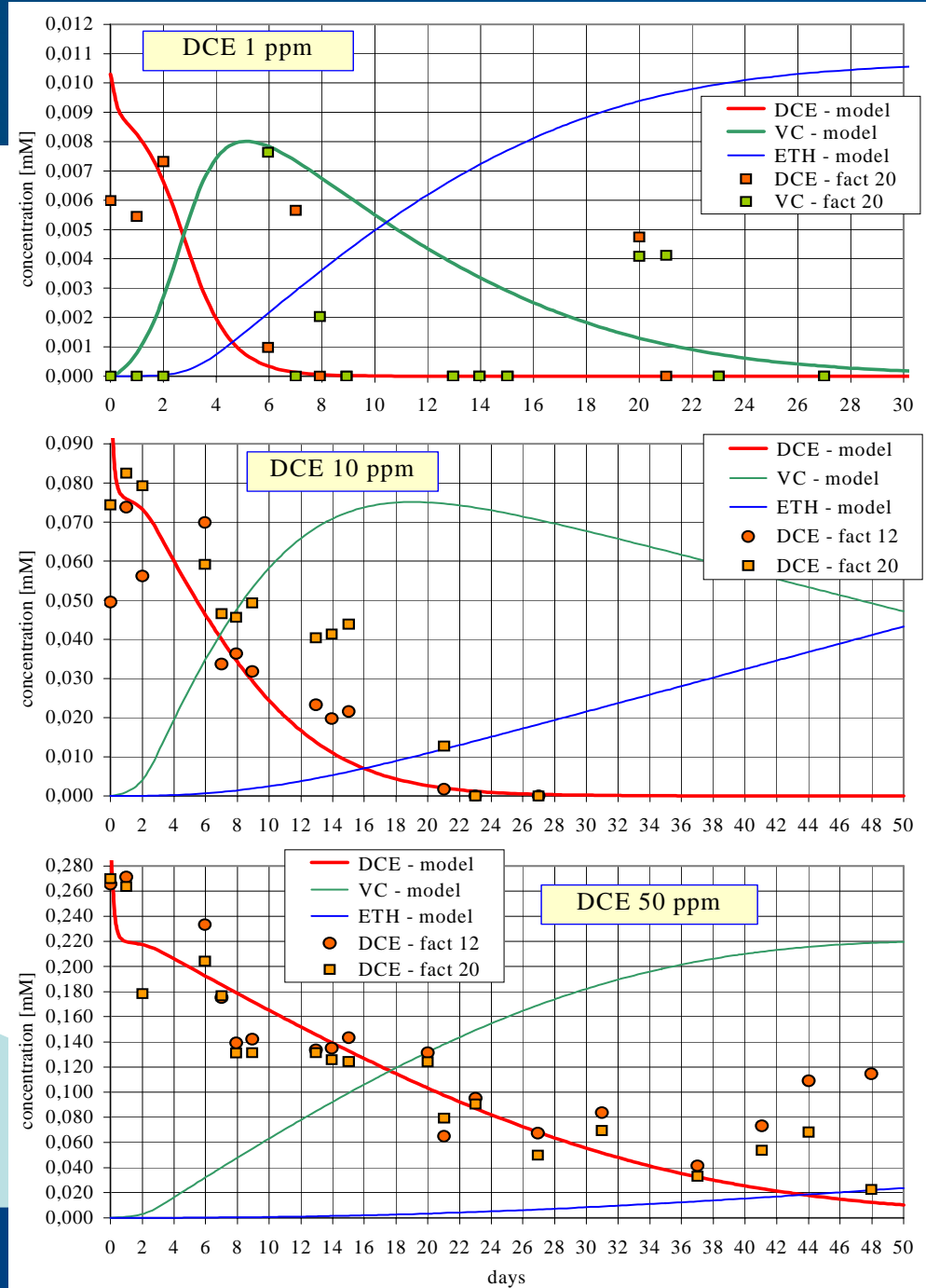
Zenne / VC Degradation



Bela Site

DCE degradation in sediment MP1

$$X_0 = 100 \mu\text{g/L}$$



CAH-Modeling

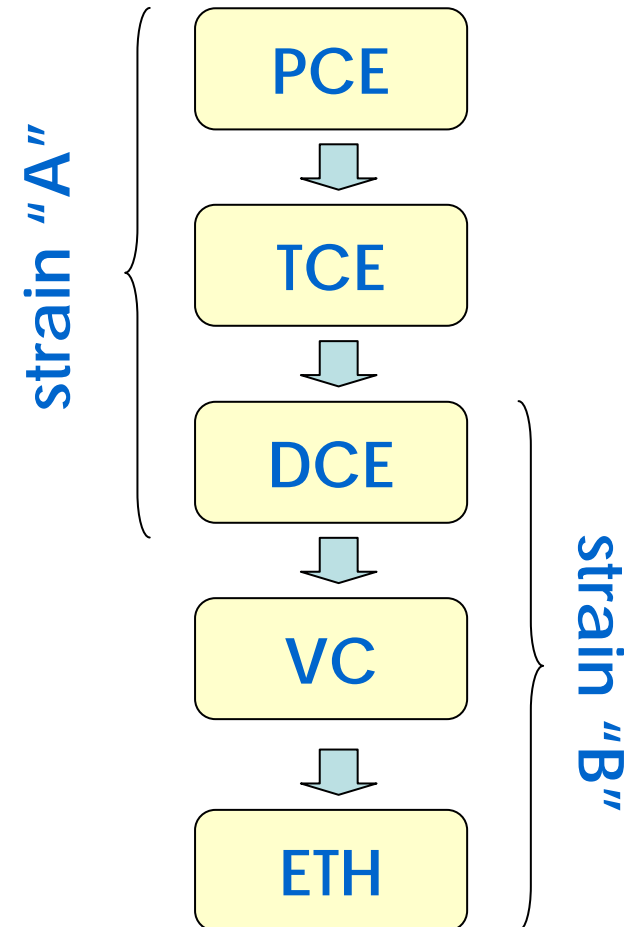
BATCH TEST

The complete
degradation chain

PCE Degradation

What is new ?

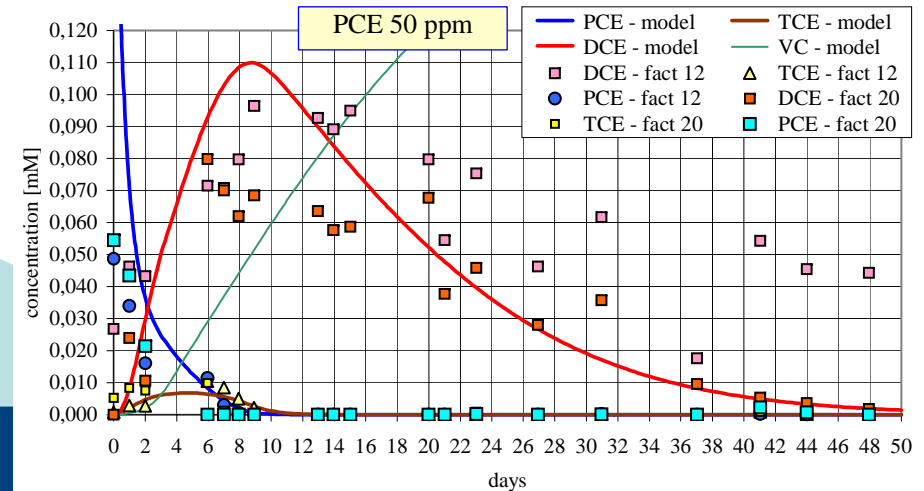
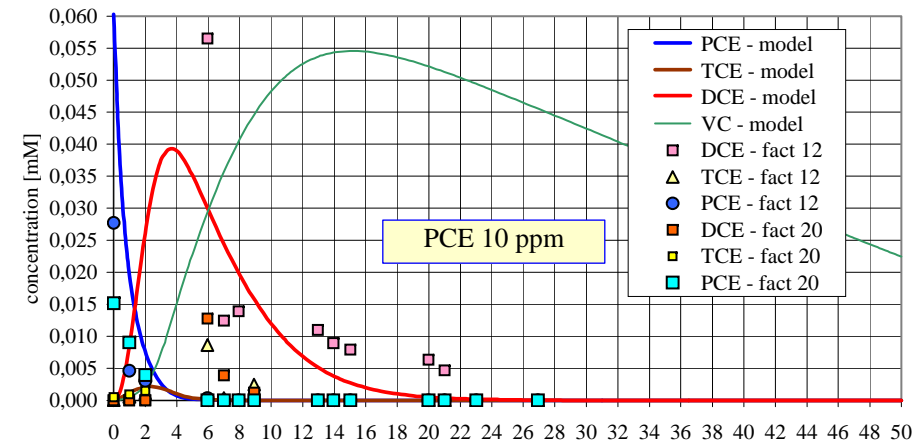
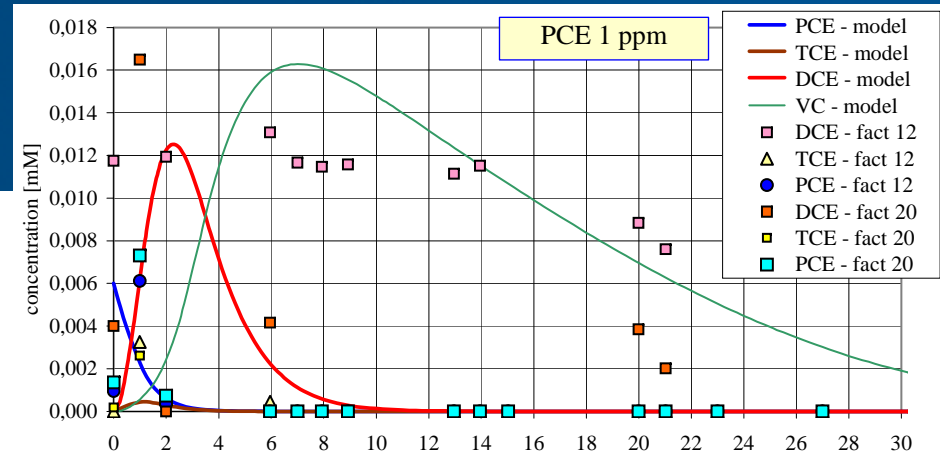
1	Strong Adsorption
2	Two Strains



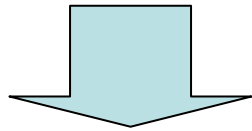
Bela Site

PCE degradation in sediment MP1

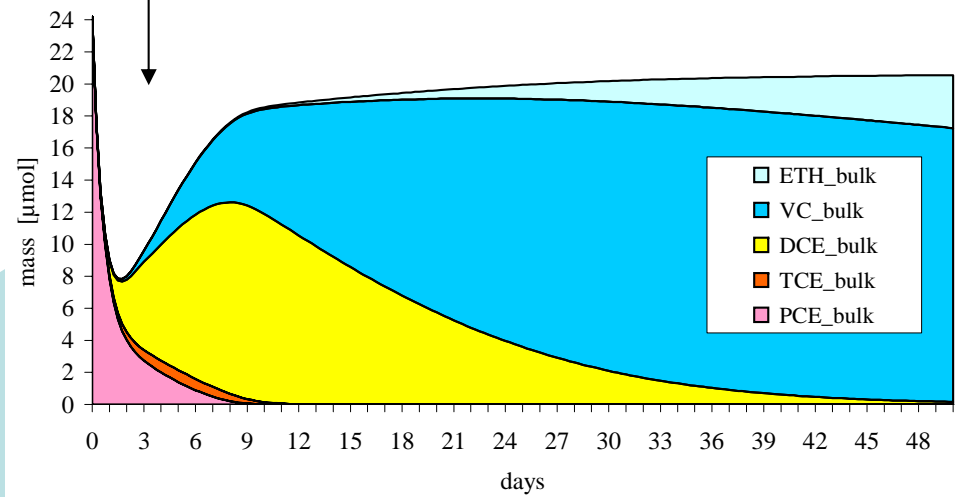
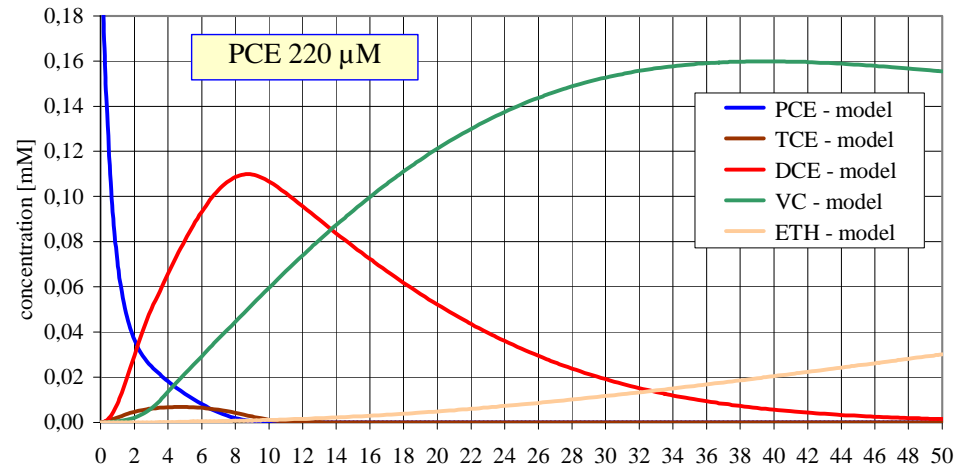
$$X_0 = 2\,000\ \mu\text{g/L}$$



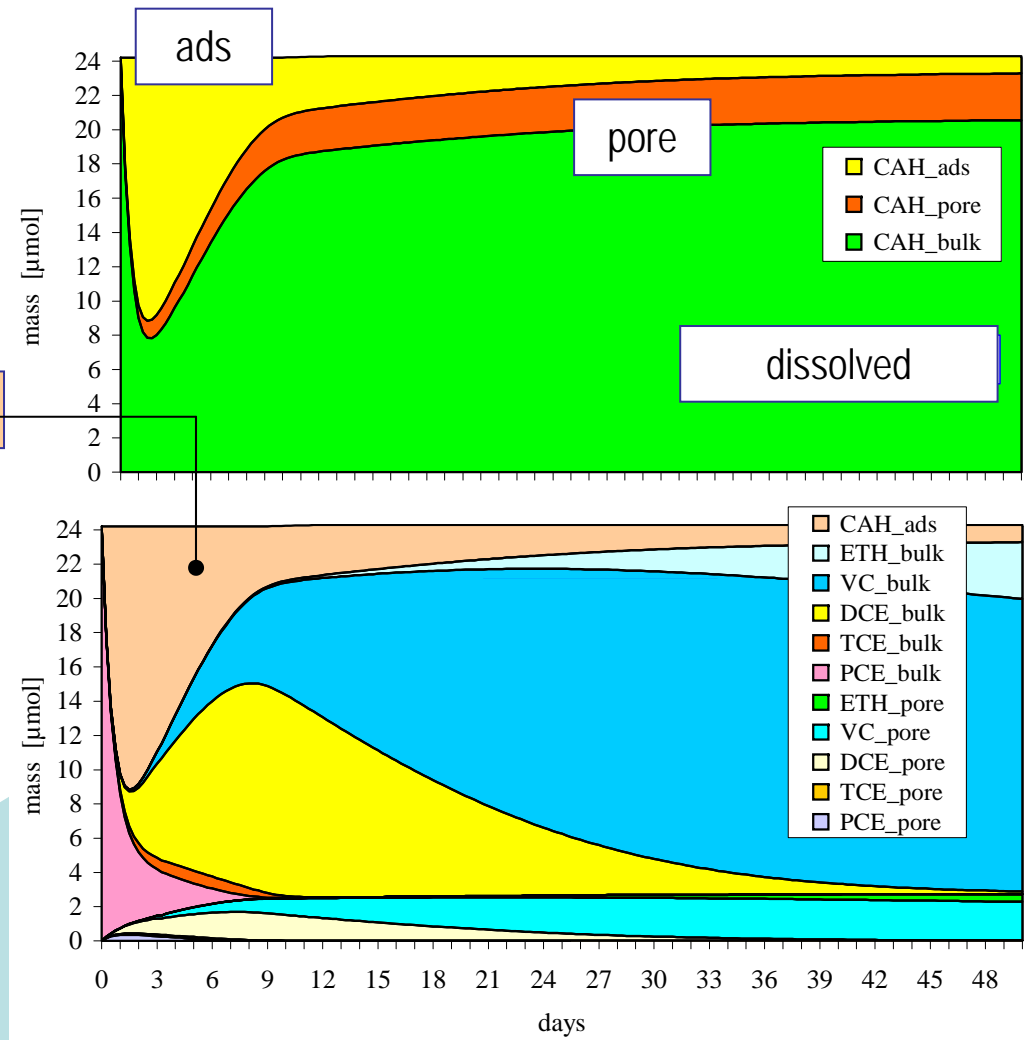
Ignoring Adsorption



Mass Balance Violation ?



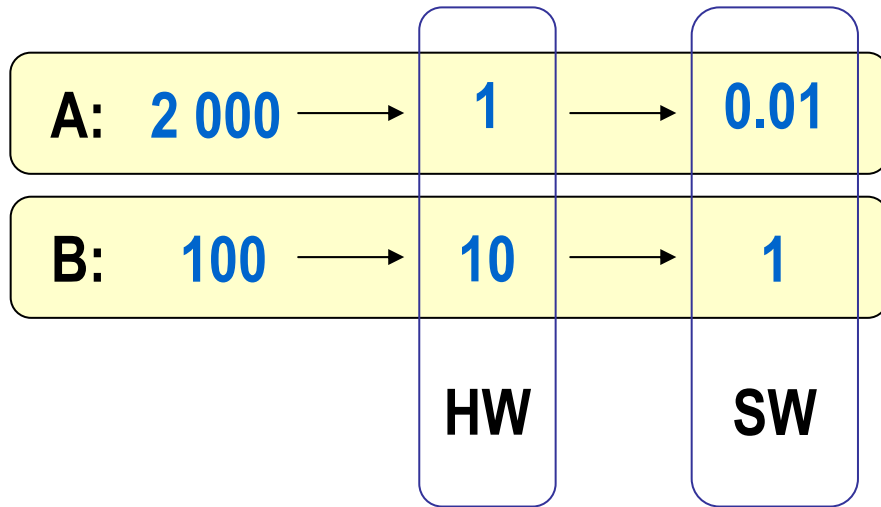
Mass Balance for PCE Degradation



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

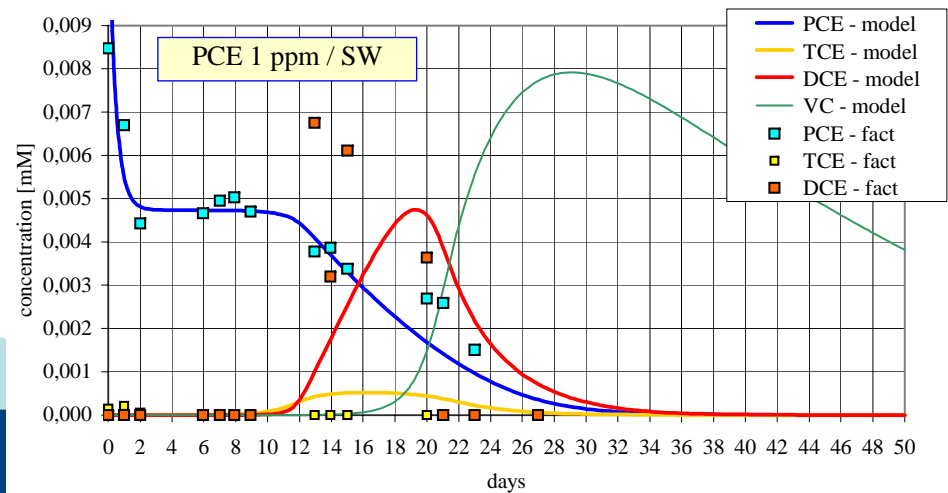
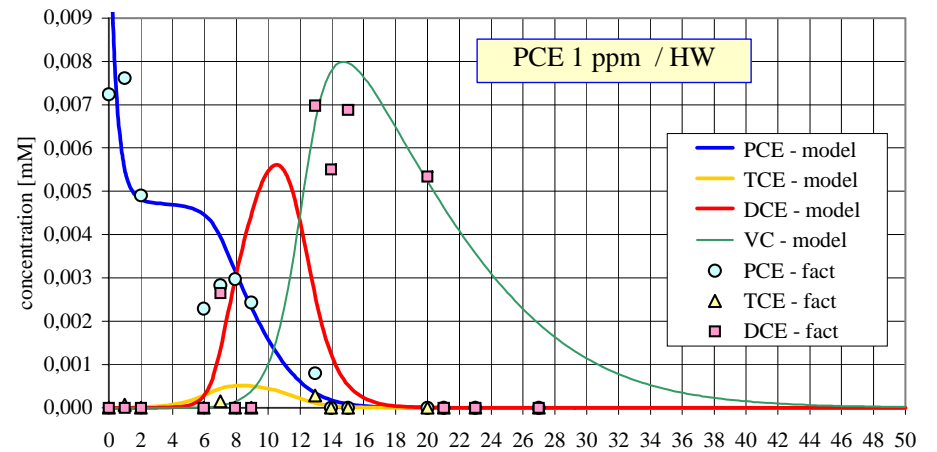
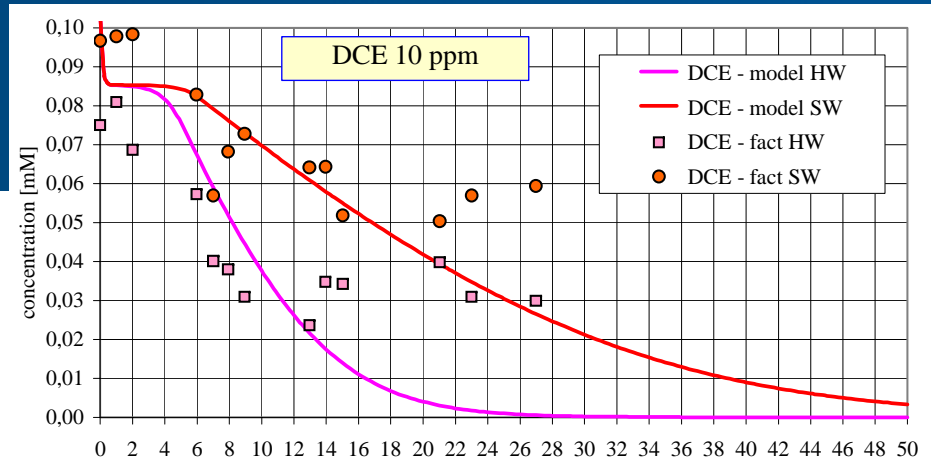
Autoclaved Sediment

groundwater surface water

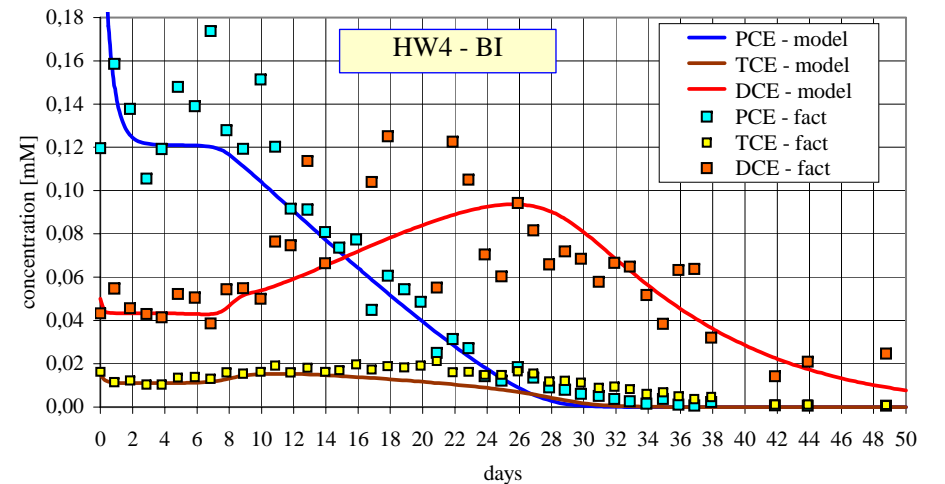
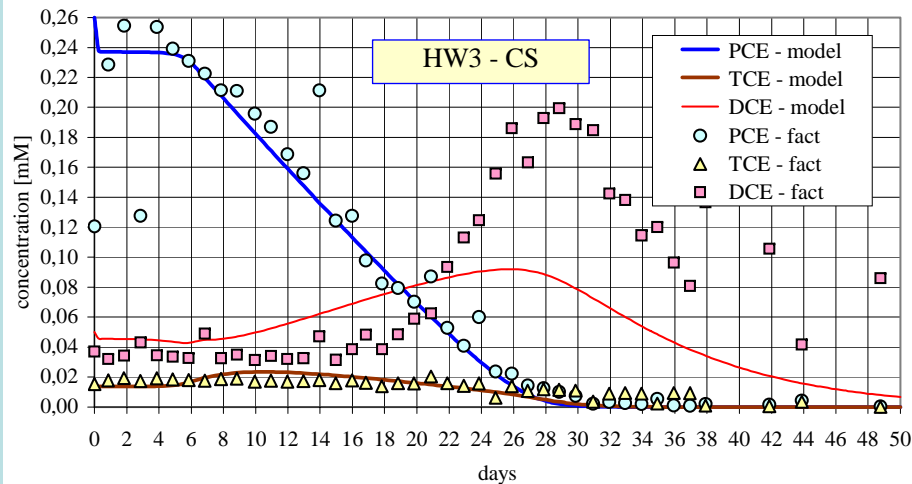
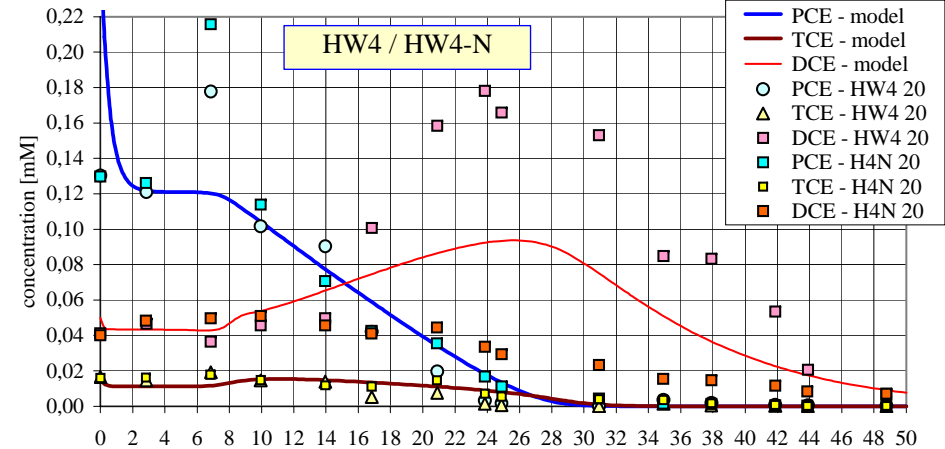
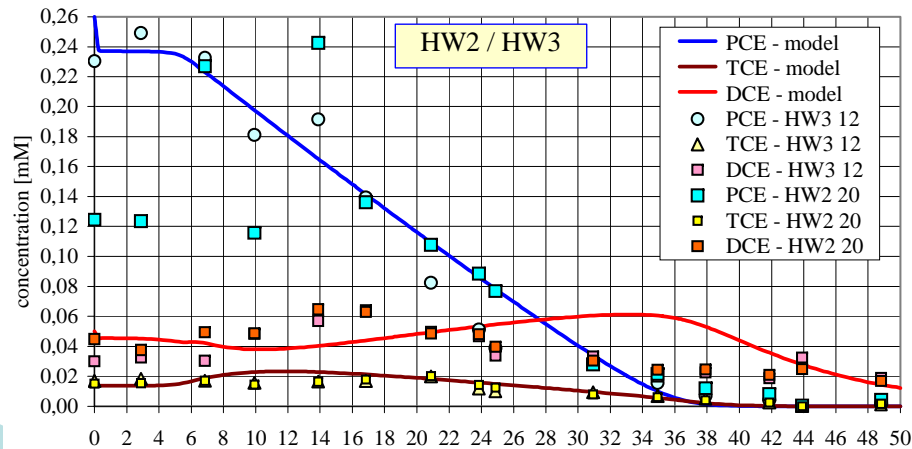


X_0 in $\mu\text{g/L}$

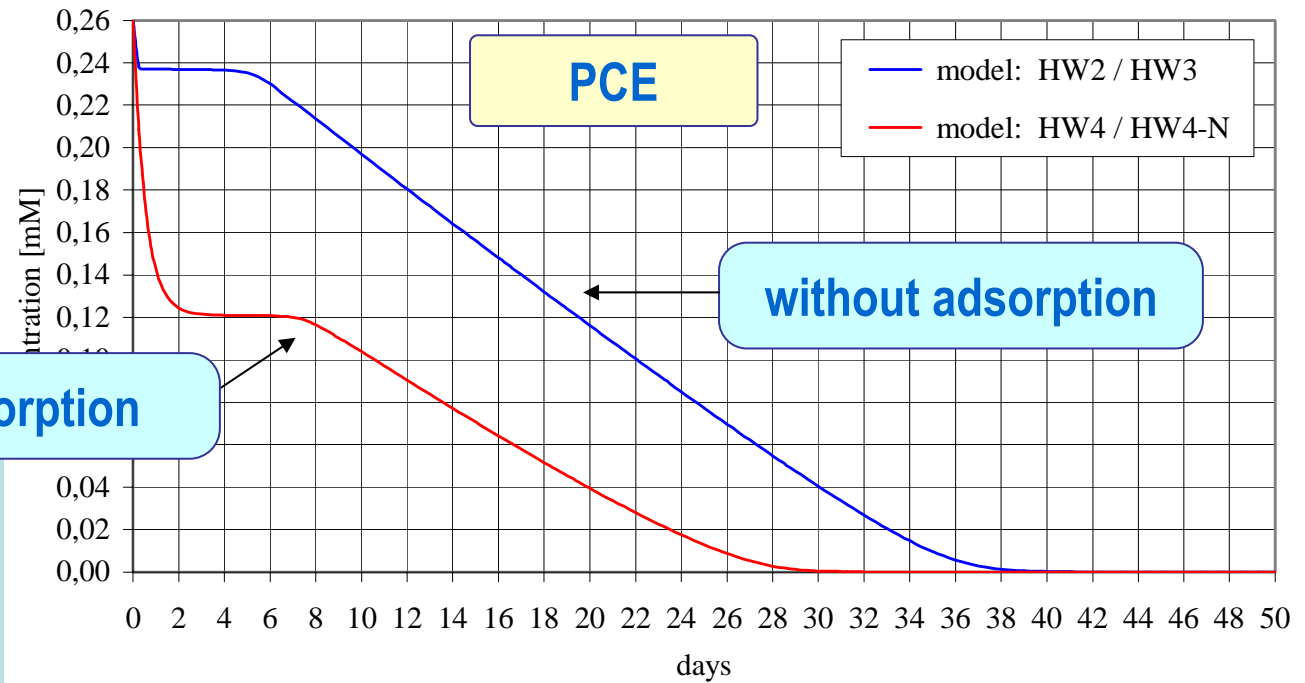
January 2006



Bela / Aquifer Material



Bela / Aquifer Material



$$X_0 (\text{aquifer}) \ll X_0 (\text{sediment})$$

CAH-Modeling

COLUMN TEST

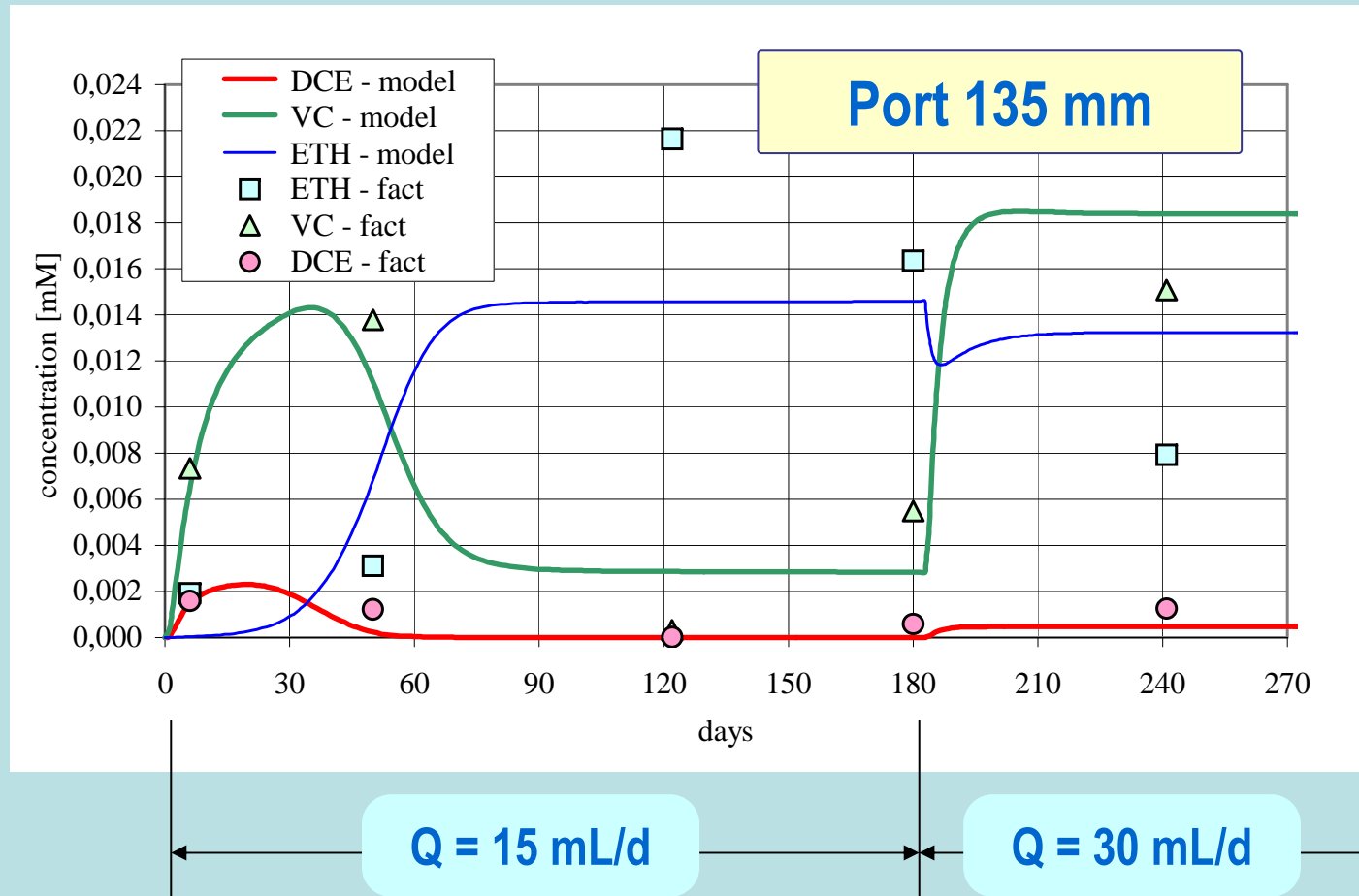
Overview

Geometry and Material Parameters

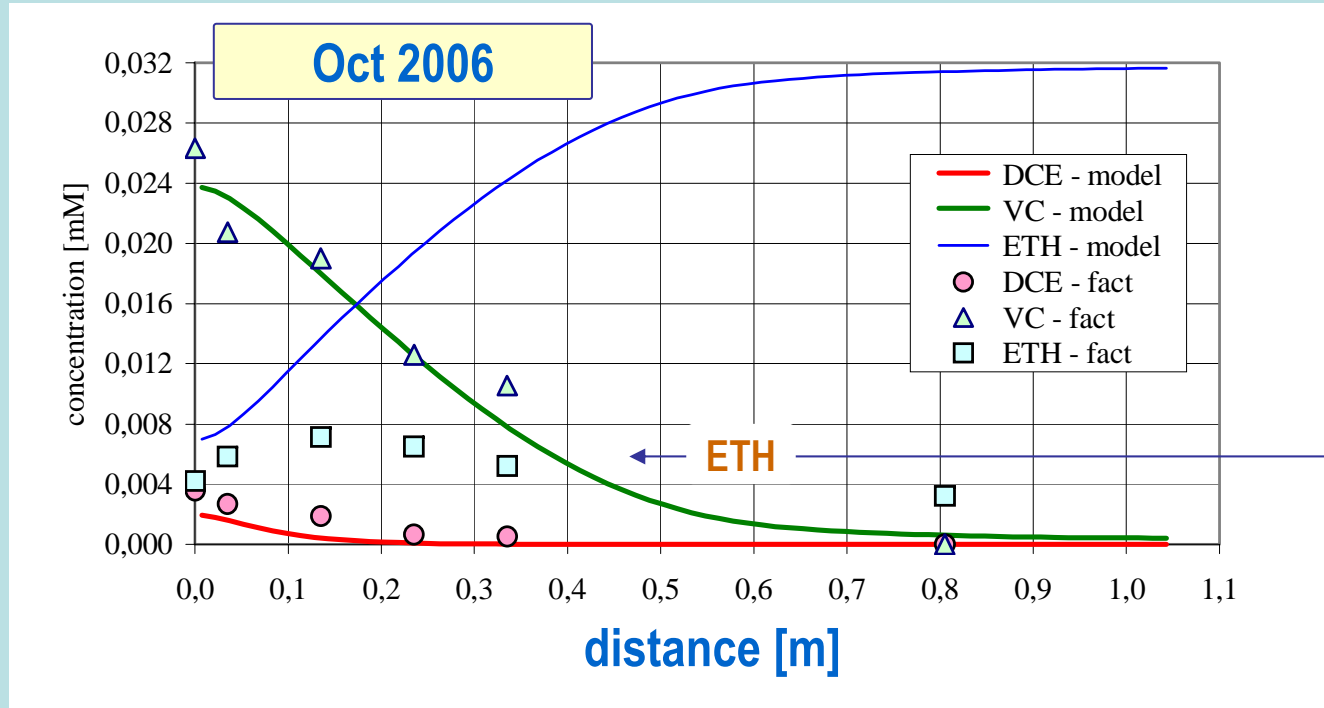
parameter	symbol	unit	Zenne	Bela
column length	L	cm	105	50
cell length	Δx	cm	1.5	2.5
cell number	$N = L/\Delta x$	-	70	20
inner diameter	d	cm	4.2	3.8
cross section	$A = \pi d^2/4$	cm ²	13.85	11.34
porosity	ε	m ³ /m ³	0.40	0.31
cell volume	ΔV	cm ³	20.8	28.4
pore volume	$\Delta V_{\text{pore}} = \varepsilon \Delta V$	cm ³	8.3	8.8
flow rate	Q	mL/d	15	226
time step (advect.)	$\Delta t = \Delta V_{\text{pore}}/Q$	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



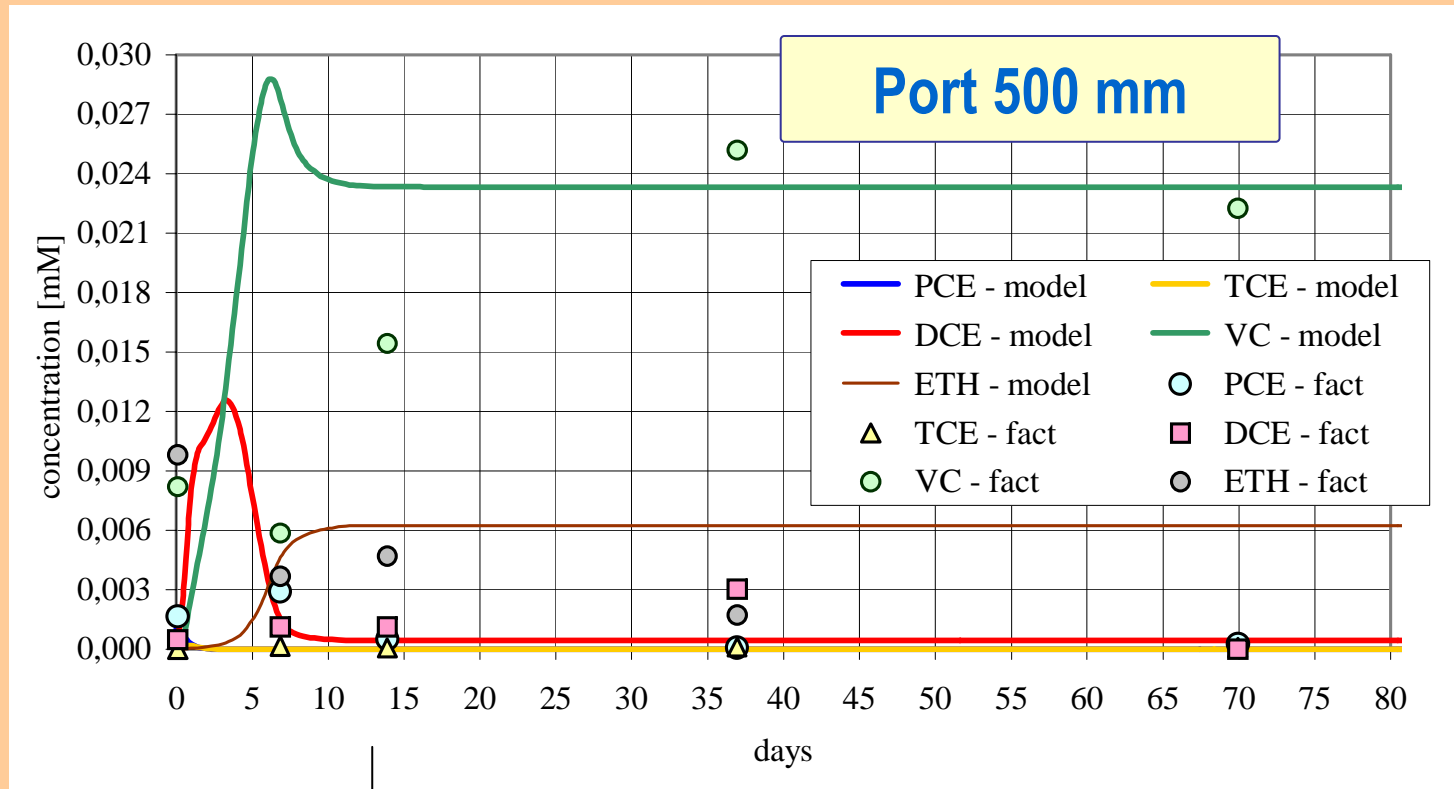
Zenne / Sediment Columns



mass balance ?

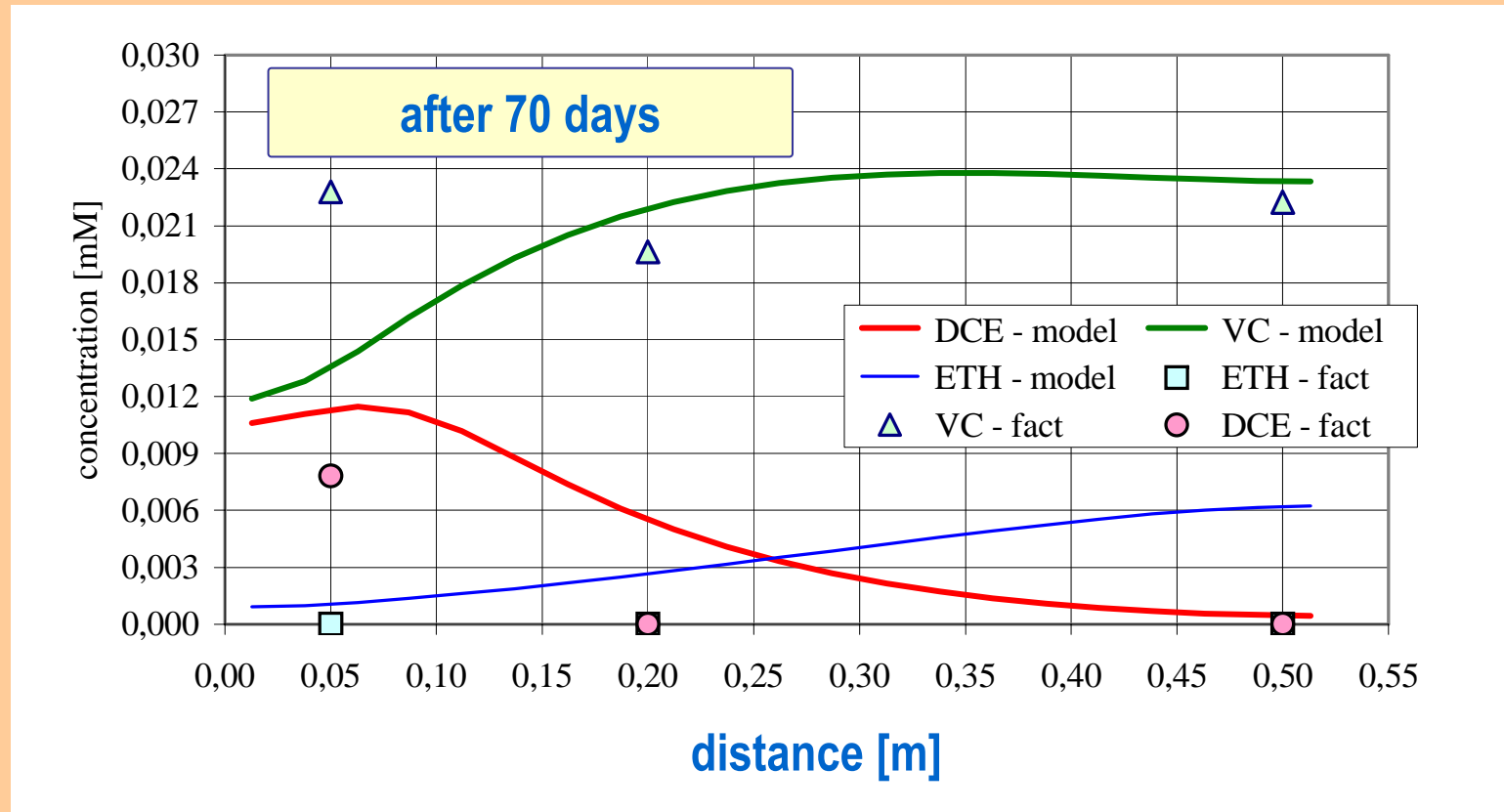
Profile

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	$Y = 18 \mu\text{g}/\mu\text{M}$
columns	$Y = 10 \mu\text{g}/\mu\text{M}$

$$\Gamma = 0.005 \text{ day}^{-1}$$

CAH-Modeling

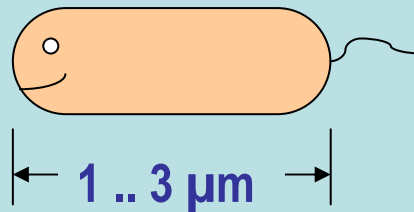
CALCULATING CFU's

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

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

biomass per Liter
pore water [$\mu\text{g/L}$]

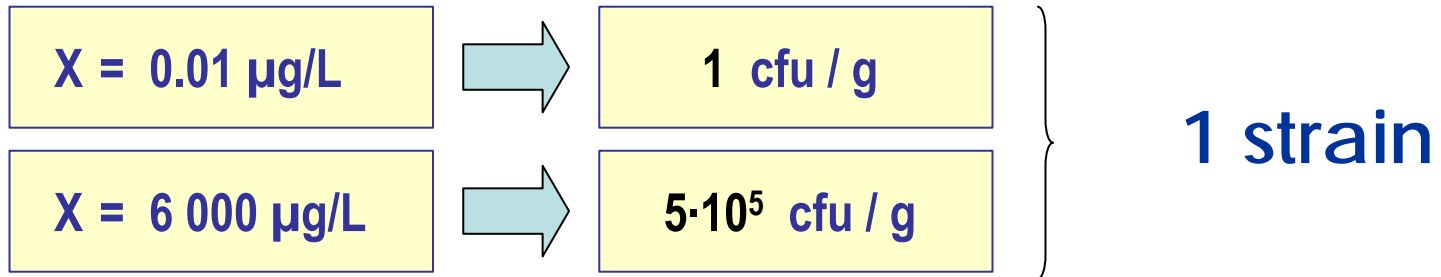
Bacteria cell



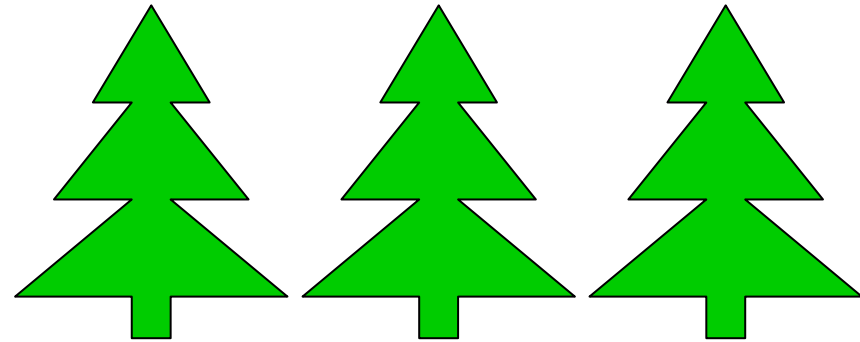
$$m_{\text{cell}} = 1.2 \text{ g/cm}^3 \cdot 2.5 \mu\text{m}^3 = 3 \cdot 10^{-6} \mu\text{g}$$

Microbial Diversity

Model



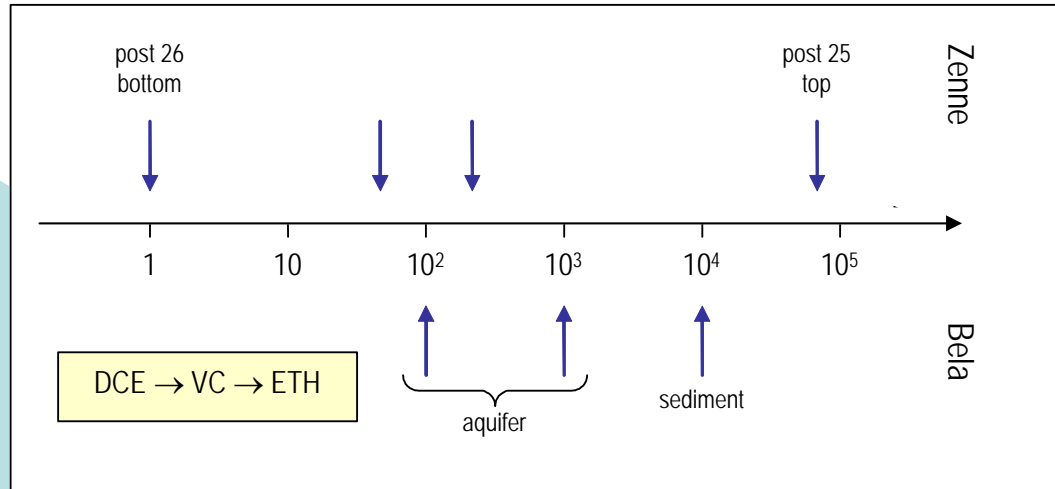
subsurface



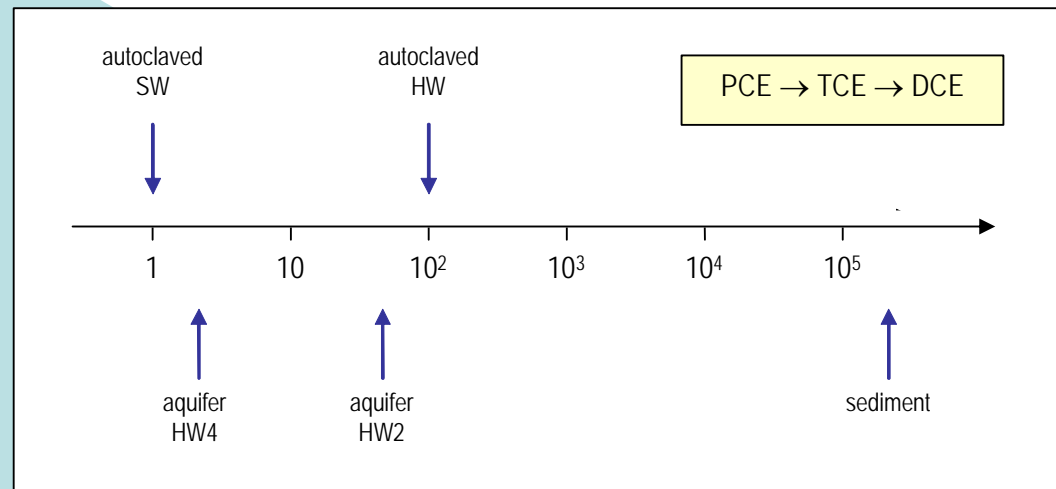
10 000 species

culturable: $10^6 \dots 10^8$ cells/g
(total: 10^{10} cells/g)

Model Results: CFU/g



initial
population

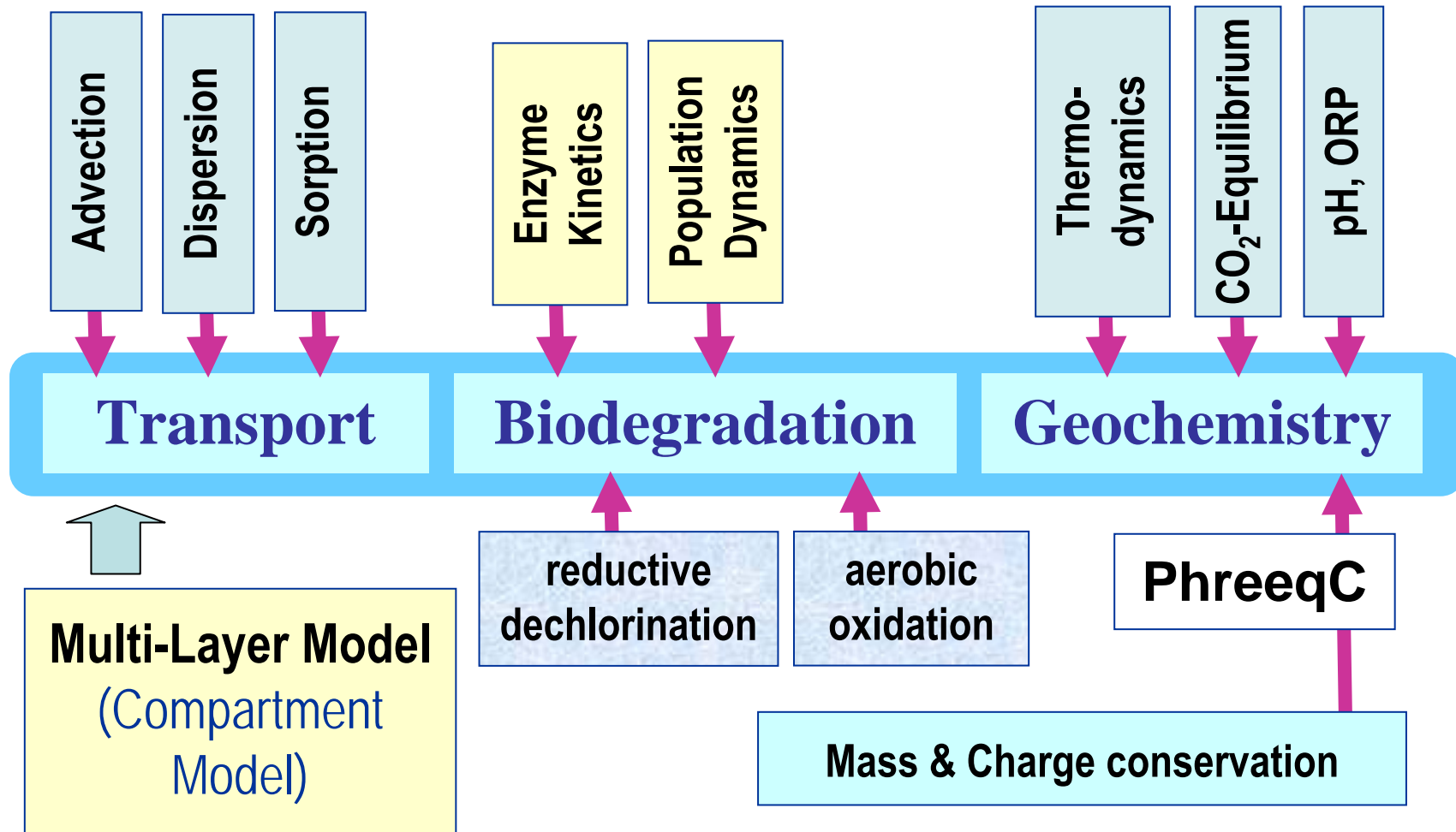


CAH-Modeling

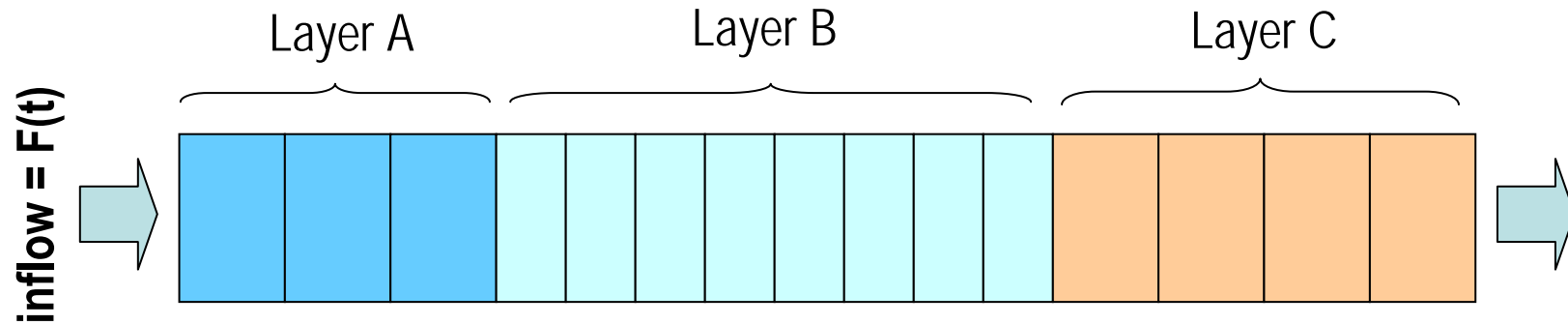
PROGRAM CAPABILITIES

January 2007

“Between-the-Discipline Model”

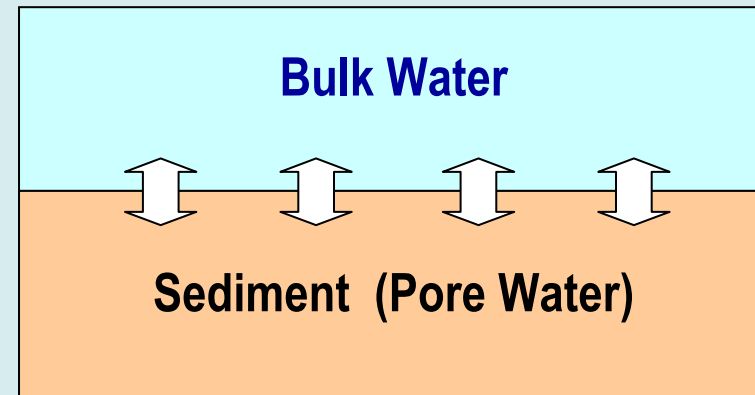


Two Options of the CAH-Model



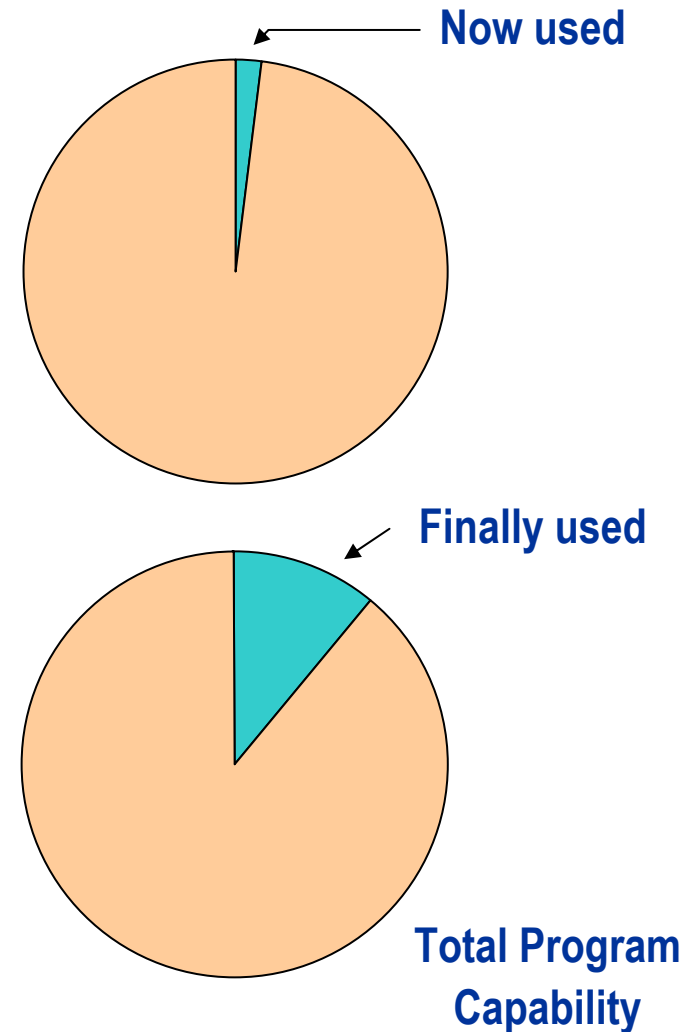
Reactive 1D-Transport

**Batch Test
(Kinetics only)**



Dynamical-Model Capabilities

	D12	D13
Enzyme Kinetics	Population Dynamics	X
	Anaerobic Pathway	X
	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	

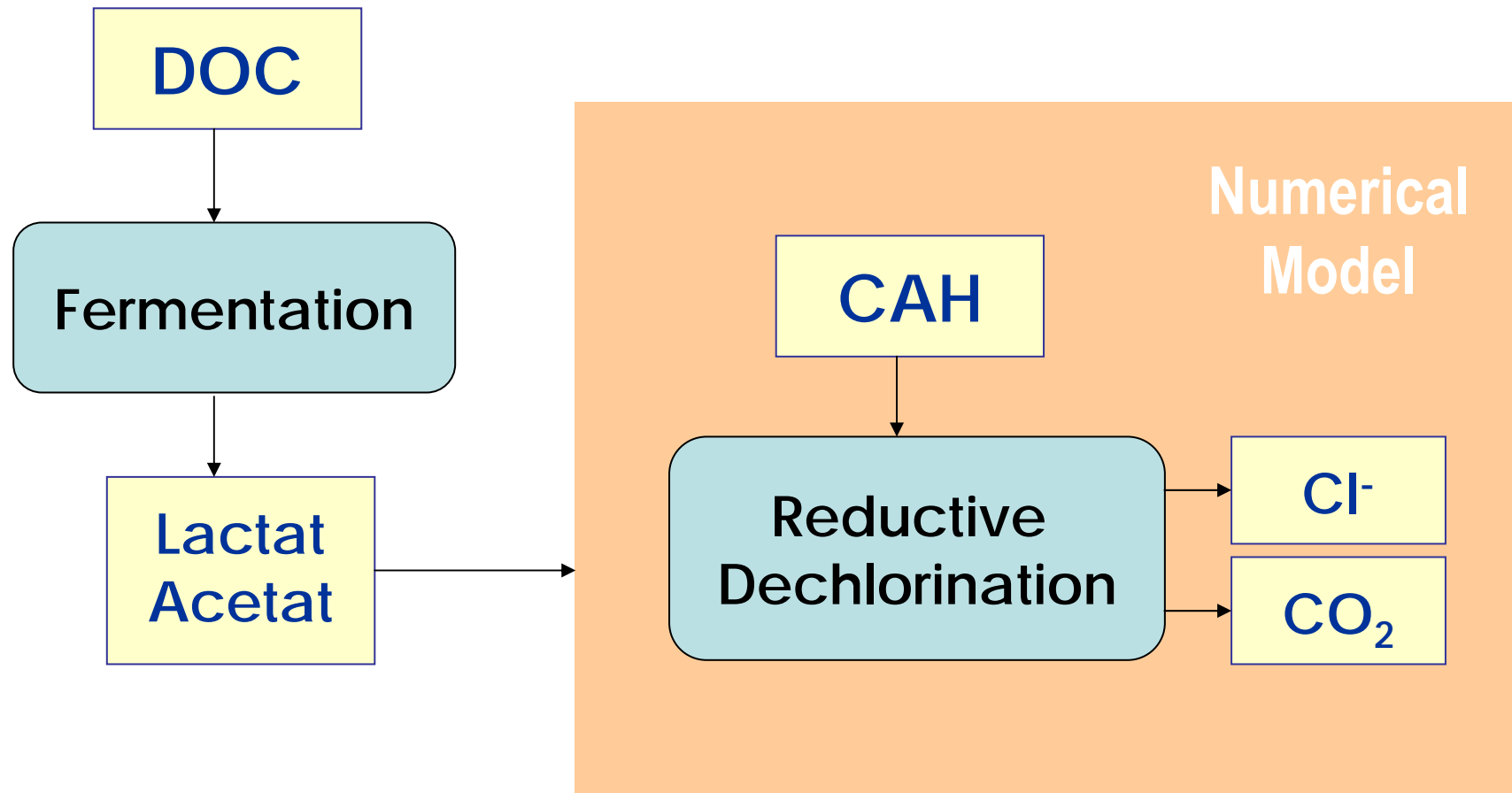


CAH-Modeling

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 !

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

Source Code

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
“Quantitative 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/cm ³	m ³ /m ³	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

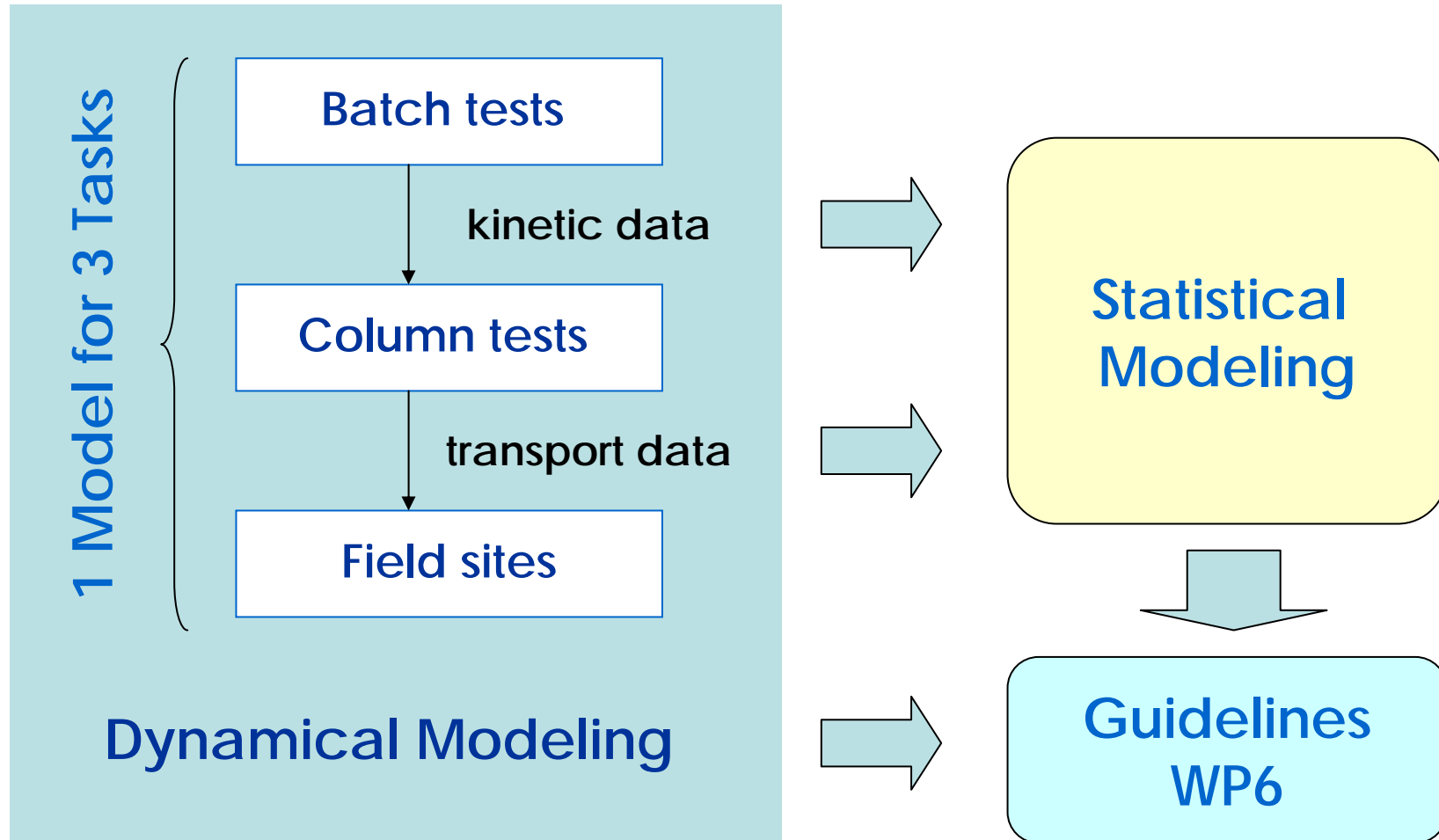
Deduced **CFU's** are in accord with other estimations

OUTLOOK - Future Model Extensions:

Symbiosis of fermentative and respirative bacteria

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

Modeling in WP5



SEDBARCAH Computer Program

Reactive Transport --- version 0.39

new start
 continue

dT [h] 3.00
 T [h] 1200

Chem without PhreeqC
 Chem with PhreeqC

kCHM 1
 kOUT 1
 kOUX 2

N cell = 40
 steps = 400
 T [PV] = 10.0
 area [m2] = 0,001385

with Dispersion
 with Adsorption
 with Reaction
 Population Dynamics
 with Ion Exchange

SEDBARCAH 2006

Input Directory: INP_03
 From Output Directory:
 To Output Directory: OUT

Graphics
 Run
 End

User Interface

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

Online Graphic

PCE
 TCE
 DCE
 VC
 ETH
 Sum

7.4%
 9.4%
 2.7%
 3.6%
 14.6%
 13.3%
 15.6%
 26.5%

Online Visualization

Time Dependence

Parameter C40_solu C40_pore inp out
 temp 0 0 0 0
 pH 25 25 25 25
 pE 7 7 7 7
 Hion -4 -4 -4 -4
 Cl 0 0 0 0
 Ca 0 0 0.2 0
 Na 0 0 0.1 0
 Nitrat 1 1 0 1
 Pce 1 1 0 1
 Tce 0 0 1 0
 Dce 0 0 0 0
 Vc 0 0 0 0
 Eth 0 0 0 0
 Doc 0 0 0 0
 C(4) 0 0 1 0
 Do 0 0 0 0
 HX 0 0 0 0

Space Distribution

Output

1260 min C40 ZoomReset
 Close