CORONA Screen – screeningový model pro hodnocení přirozené atenuace

Josef V. Datel

Výzkumný ústav vodohospodářský TGM, v.v.i.

jvdatel@gmail.com

datel@vuv.cz

Podklad

- Tento příspěvek byl zpracován na bázi zprávy – dílčího výstupu mezinárodního projektu CORONA z 5. rámcového programu Evropské komise:
- ***Wilson R.D., Thornton S.F., Hüttmann A., Gutierrez-Neri M., Slenders H.: Guidance for the application of NA assessment screening models. University of Sheffield, United Kingdom and TNO, The Netherlands.***

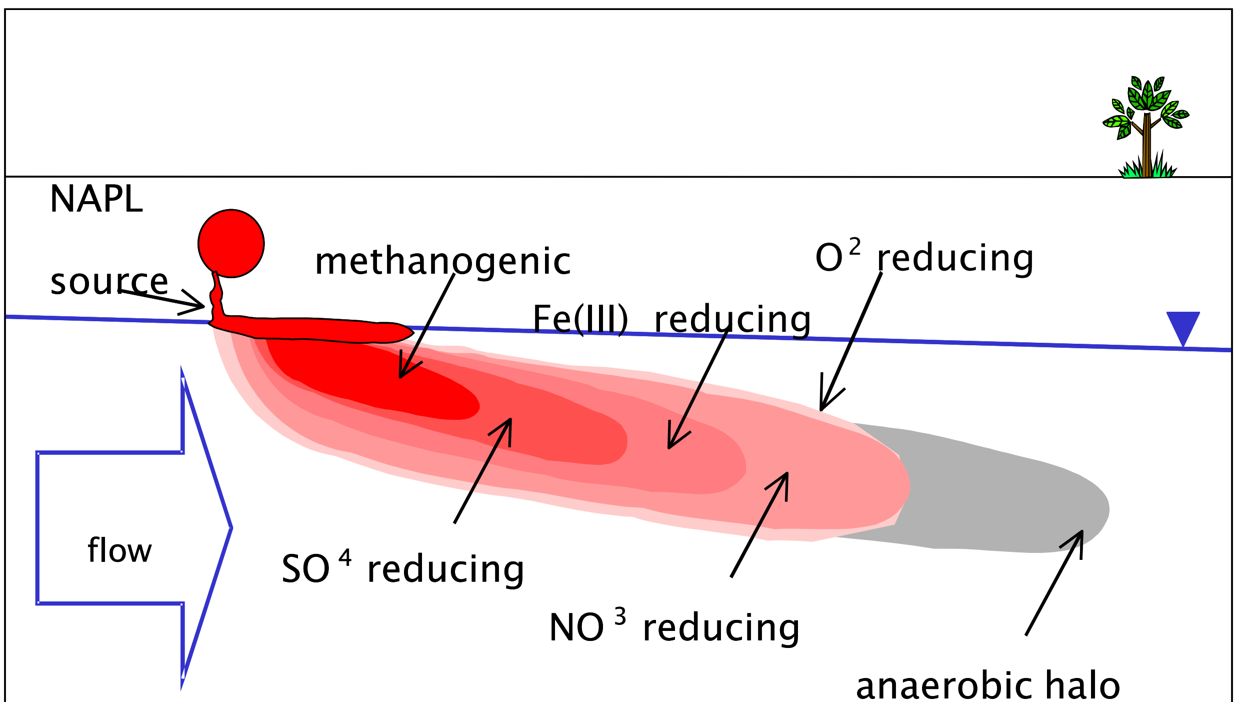
Stránky projektu

- *www.corona.group.shef.ac.uk*
- *Články, informace*
- *Prezentace*
- *Model CORONA SCREEN k volnému stažení*

The CORONA hypothesis

NA of oxidising organic contaminants:

- A common pattern of biodegradation activity can be found in most plumes
  - aerobic redox conditions at the outer plume edge grading to methanogenic at the plume core

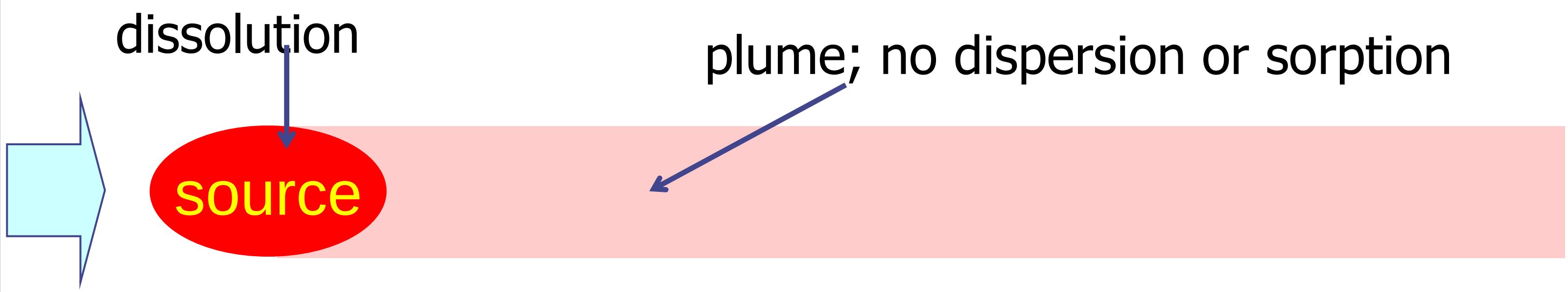


The CORONA hypothesis

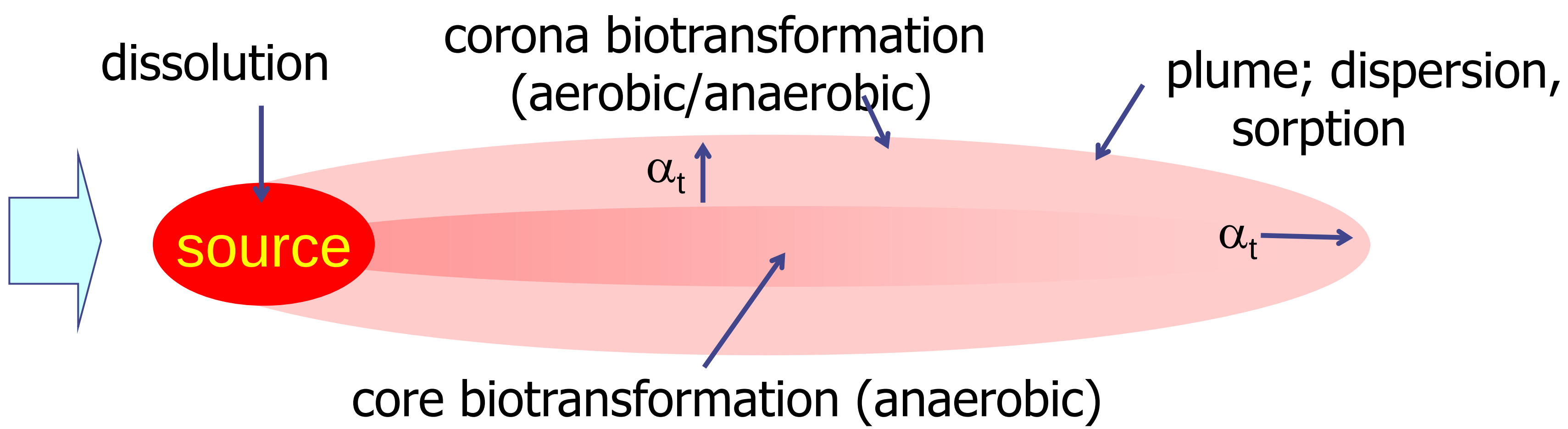
- Biodegradation in the plume fringe or CORONA zones is thermodynamically favoured
- Biodegradation in the Corona makes the most significant contribution to the overall rate of contaminant mass loss from the entire plume
- Mixing of electron acceptors and contaminants in the Corona controls maximum plume length

Conceptual model

Earliest conceptualisation – we never see this



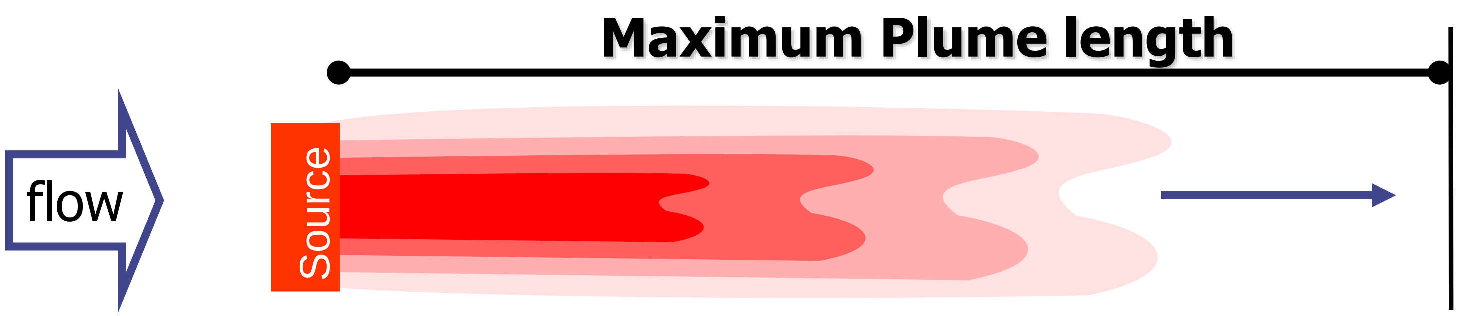
Current, realistic conceptualisation



Plume Life Phases

Growth Phase

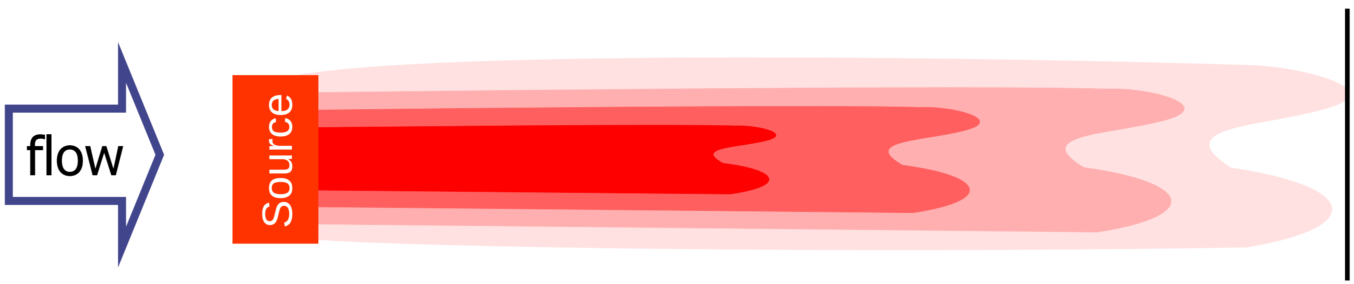
- Groundwater plume starts to form and is transported downgradient faster than rate of natural attenuation
  - Growth rate depends on groundwater velocity, sorption and biodegradation
- Growth phase ends at maximum plume length



Plume Life Phases

Steady-State Phase

- Rate of contaminant mass flux is offset by contaminant mass attenuated by natural processes
  - In the case of dissolved species it is rare that a plume will reach a steady state condition
  - NAPL sources on the other hand may last for centuries



Plume Life Phases

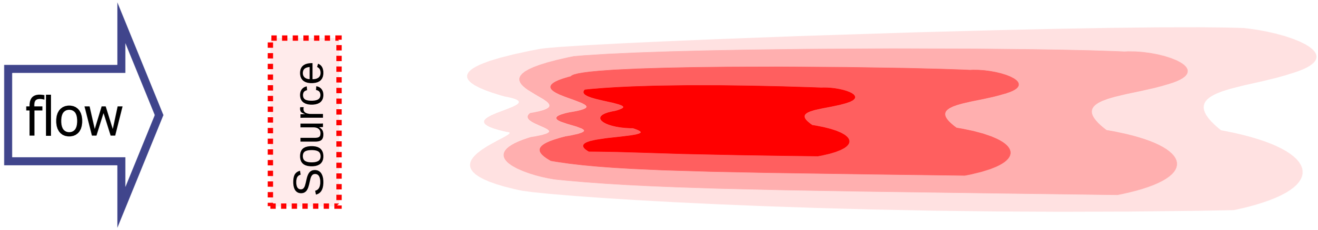
Decay Phase

- Contaminant mass flux no longer matches the rate of attenuation
  - If attenuation rate increases the plume may shrink until it achieves a new steady state
  - If the source is exhausted the plume will decay until it disappears
    - Plume may appear to shrink in length but since NA occurs everywhere it will in effect ‘dissolve’ away

Detached Plumes

No significant contaminant mass flux from the source area

- Depletion or remediation
- Plume can still move downgradient
- We can expect the plume to decay by NA processes



Screening Models

Simplified models that allow rapid NA assessment

Spreadsheet-based

- easy to use

Many assumptions

- designed to approximate

Model Application

Screening models incorporating analytical solutions of the mass transport equation have been used to explore various basic characteristics of a plume

- Assume biodegradation proceeds at a uniform pseudo rate for all electron donor/acceptor couples

Model Application

A wide range of source/plume scenarios can be approximated by analytical solution

Simplified models are easier to operate and run quicker

- Provided that they fit with the conceptual model

Screening Tools

Three screening models currently available:

- Bioscreen – For use on oxidising plumes
  - http://www.epa.gov/ada/csmos/models/bioscrn.html
- NAS – For use on oxidising plumes
  - http://ceeweb.cee.vt.edu/nas/index.html
- BioChlor – For reductive dechlorination
  - http://www.epa.gov/ada/csmos/models/biochlor.html

Screening Tools

All three models use a modified form of the Domenico (1987) analytical solution

- for a degrading contaminant plume from a vertical plane source

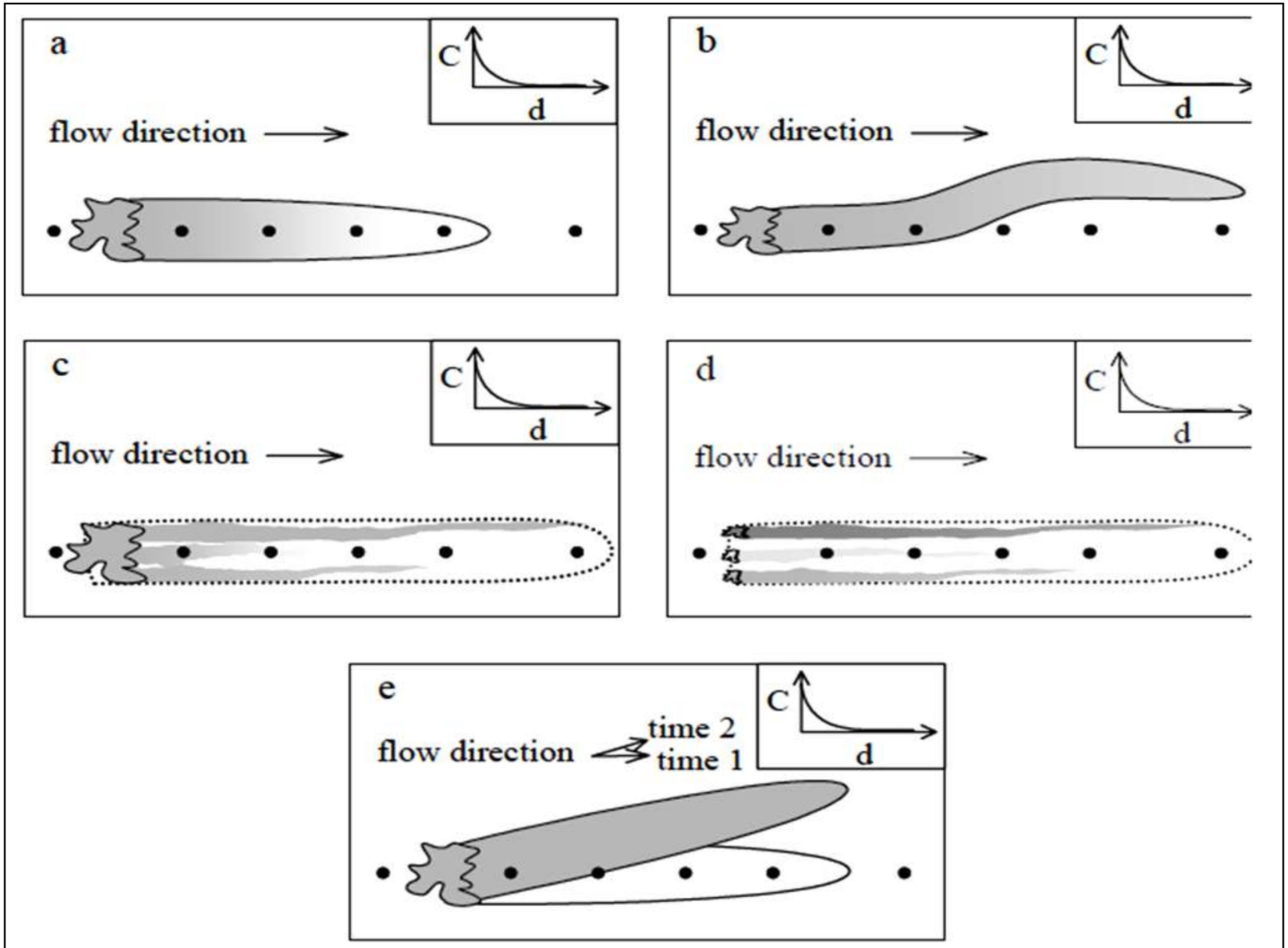
From a small number of input parameters a profile of contaminant concentrations along the theoretical plume oxidising centreline is calculated

Screening Tools

Input Parameters for BioScreen

groundwater velocity
longitudinal dispersivity
transverse horizontal dispersivity
transverse vertical dispersivity
retardation factor
1st order biodegradation constant
source area width and thickness
source contaminant concentration
background electron acceptor concentration

Rizika průzkumu v předpokládané ose kontaminačního mraku



The CORONA Approach

Does NOT seek to obtain plume centreline concentration data or gather lines of evidence

Seeks to quantify and rank the key NA processes influencing plume transport

- e.g., oxidation will be controlled by the mixing of electron acceptors at the plume fringe, controlled by vertical transverse dispersion
- Data collection would be designed to allow estimation of dispersivity, inward electron acceptor flux gradients and outward contaminant flux gradients

Core and Fringe Controlled Plumes

Focus on process identification and quantification allows determination of where within the plume the majority of contaminant biodegradation occurs

- Fringe processes control plume attenuation where contaminants are oxidised
- Core processes control plume attenuation where contaminants are reduced e.g. chlorinated solvents
- In some cases both may contribute

Multilevel Wells Methods

High-resolution multilevel wells should be installed

- Allows quantification of dispersive electron acceptor and plume gradients at the plume fringe

Focus on process quantification rather than spatial contaminant distribution

- Possible to make reasonably accurate estimates of NA from fewer wells

Monitoring strategies – well design

Long screened wells

- depth averaged concentrations
  - no vertical process resolution

Nested short screened wells set at different depths

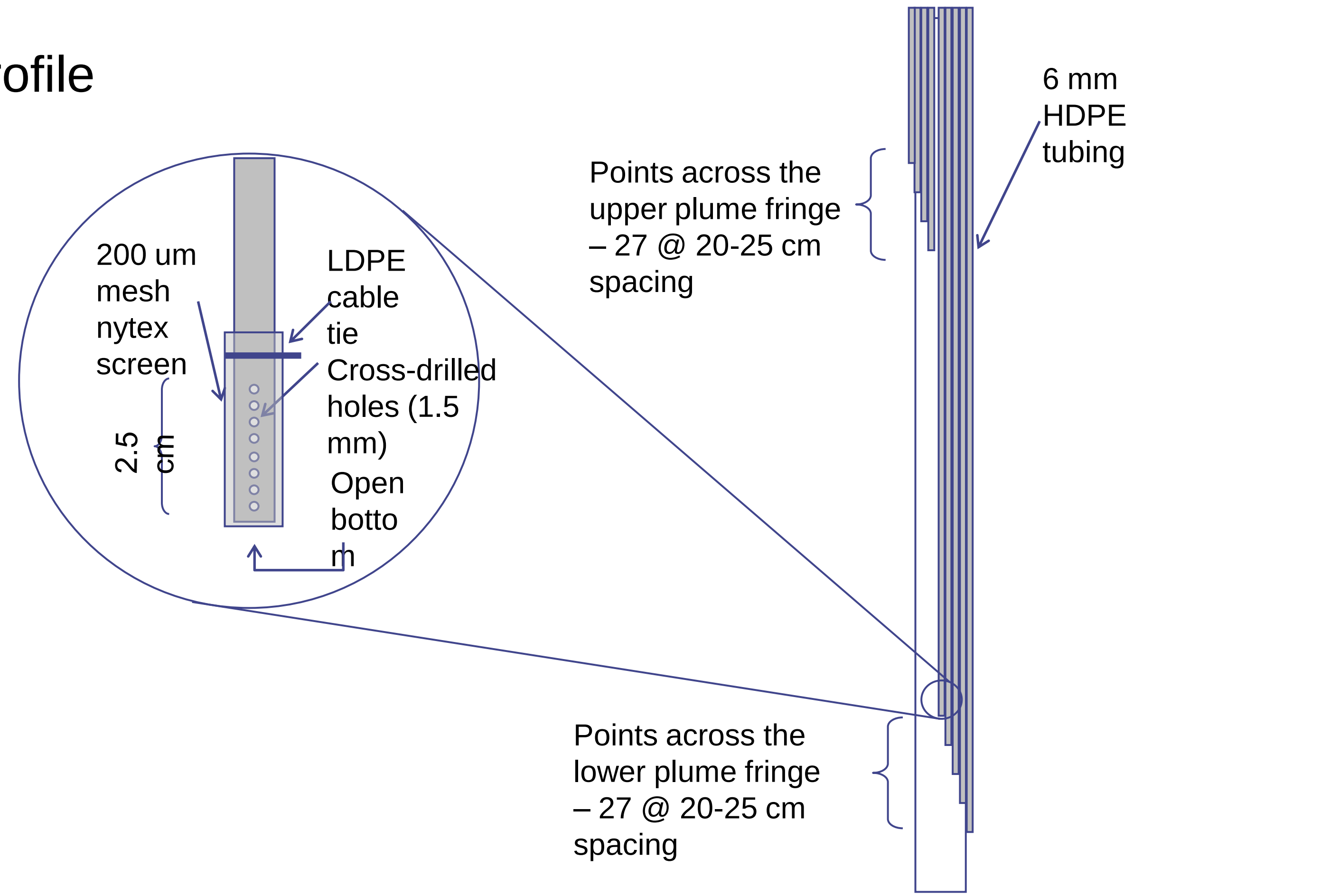
- more discrete vertical data
  - poor vertical resolution

Multilevel wells

- variable vertical resolution

ML Construction

profile



Confounding Effects of Heterogeneity

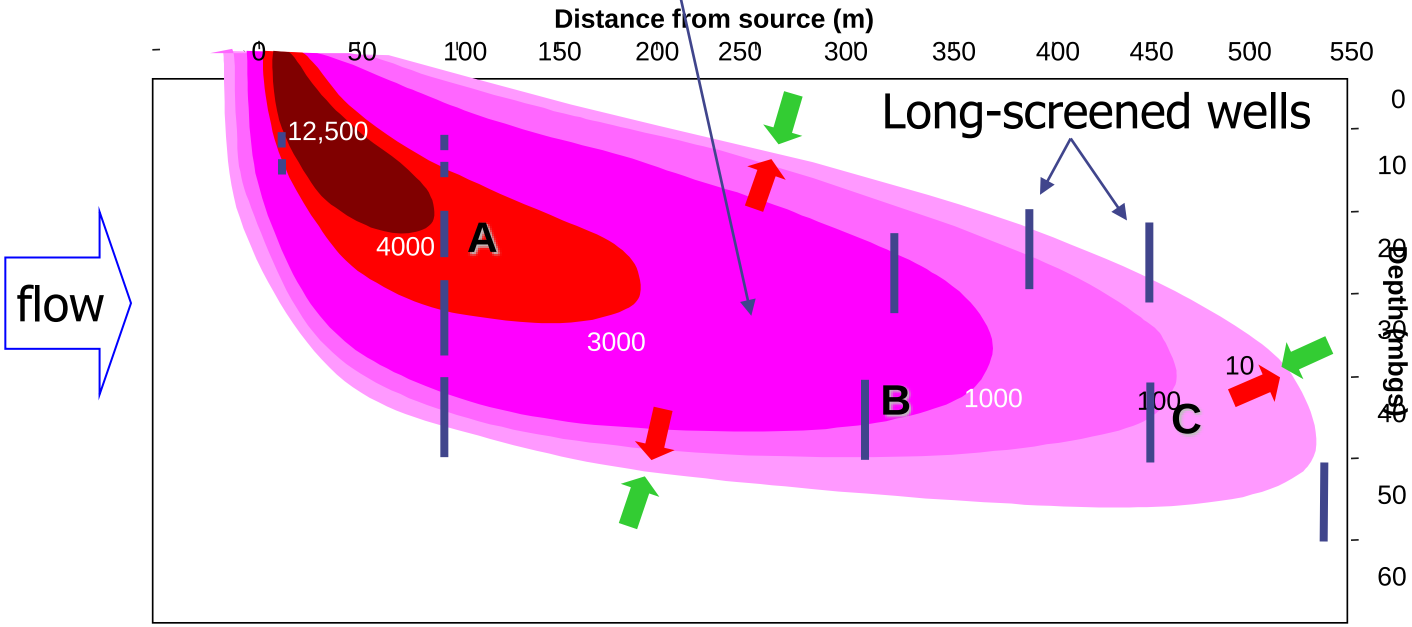
In many cases aquifer heterogeneity results in:

- Spatially variable source distribution
- Contaminant flux along preferred paths
  - Resulting in plumes that lack a unique centreline
  - Using data from wells that do not represent a centreline can lead to over/under representation and a high degree of uncertainty

A site conceptual model based on long-screened monitoring wells

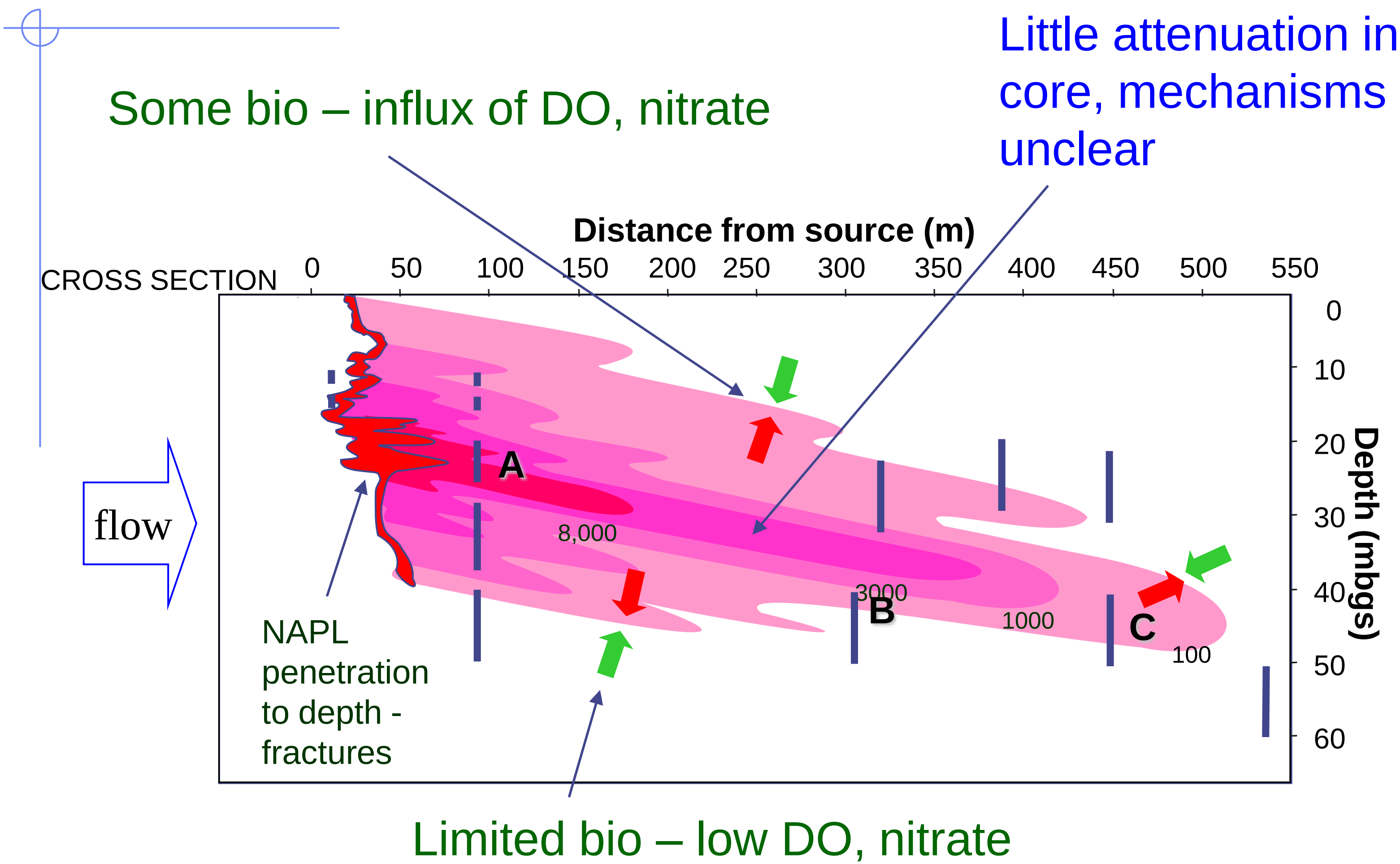
CROSS-SECTION

Fermentation in the plume core



Fringe mixing of contaminants and electron acceptors

Updated site conceptual model



Monitoring Strategies

Type

High resolution multilevel samplers

- resolve vertical electron donor and acceptor diffusive flux gradients
- resolve vertical dispersive mixing

Location

At least one near source

- ideally another downgradient

CoronaScreen

Based on the hypothesis that

"The identification and quantification of key NA processes will yield a better NA assessment than spatial concentration data"

Existing Site Data

Dispersivity

- tracer tests
- inverse modelling

Source geometry

- site investigation

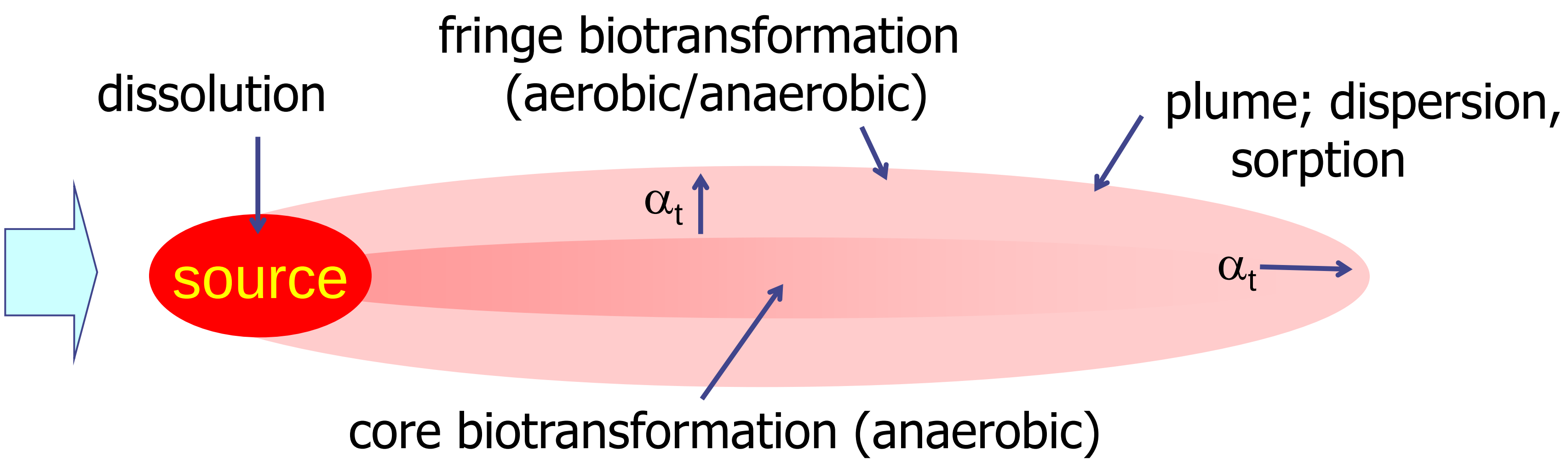
Source strength

- sampling (temporal and spatial)

What Do We Need to Know to Make a Decision?

What's the maximum plume length?

What processes are controlling NA in the plume?



Key Parameters

Input requirements are generally limited to:

- Groundwater velocity
- Source geometry (Area x Depth)
- Source concentration
- Electron acceptor concentrations
- Longitudinal and/or transverse dispersivity

Philosophy of Modelling

Approximation of NA

- maximum plume length (L)
- time to reach L

Early decision making

Identification of key NA parameters

- match to screening model confirms dominance of key parameters

CORONA Screen Model

www.corona.group.shef.ac.uk

Features

processes, rather than centreline data

instantaneous biological reactions

- assume reactions faster than transport flux

stoichiometric conversion of all Electron Acceptor/Electron Donor concentrations to electron equivalents

- simplifies chemistry to:
  - combined electron donors
  - combined electron acceptors

Plume Development Prediction

- maximum plume length
  - key NA decision-making parameter
- time to steady state
  - important for site management
- concentration at compliance point

Critical parameter identification (sensitivity)

Outputs of CORONA EU project

- study of 1 lab + 6 field plumes
  - identification of NA-controlling parameters
  - quantify dispersivities
  - inverse numerical modelling
- Scenario modelling
  - idealised cases

Benefits and Limitations

Benefits

- easy to run
- few input data required

Limitations

models are simplifications

- can’t handle complex biochemistry

oxidisable contaminants only

The CoronaScreen Model

- 3 models, each using a different conceptual approach
  - same goals and outputs
- provides independent NA assessment
  - internal verification
- Excel-based

The Three Component Models

travelling 1-D

- vertical 1-D dispersive transport

analytical

- modified Domenico (1987) analytical solution

electron balance

- flux balance of electron acceptors/donors at all plume boundaries

Nároky na vstupní parametry

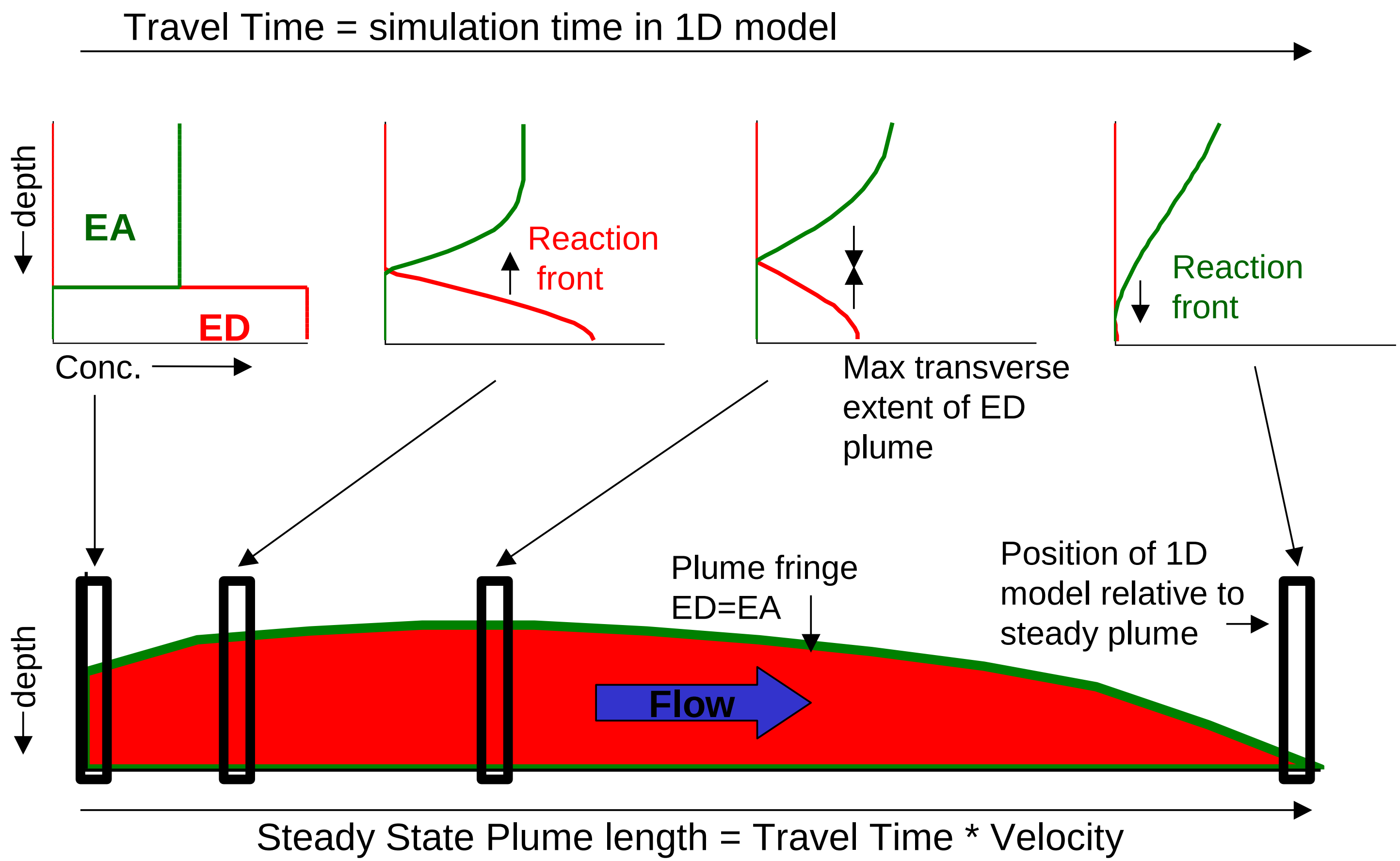
Parametr	1-D transportní model	Analytický model	Model elektronové bilance
Rychlost proudění podzemní vody	x	x	x
Vertikální disperzivita		x	x
Horizontální disperzivita		x	x
Podélná disperzivita		x	
Šířka kontaminačního mraku		x	x
Tloušťka kontaminačního mraku		x	x
Tloušťka okrajové reaktivní zóny		volitelné	x
Pozaďové koncentrace elektronových akceptorů*	x	x	x
Koncentrace elektronových akceptorů* v mraku	x	x	x
Pozaďové koncentrace elektronových donorů**	x	x	x
Koncentrace elektronových donorů** v mraku	x	x	x
Pórovitost			x
Měrná hmotnost horniny			x
Frakce organického uhlíku			x
Vzdálenost vzorkovacího vrtu od zdroje znečištění		x	

Travelling 1D

A 1D travelling transverse model for simulating steady state plume profiles

- Uses PHREEQC to dispersively mix a 1D column of water
- Orientated transverse to plume to predict the plume's steady state profile
- By simulating the transverse dispersion and reaction the 1D model predicts the time taken for mass leaving the source area to be completely consumed

Travelling 1-D schematic



What It Does

Allows rapid estimation of plume lengths

Uses initial conditions equivalent to assumed continuous source of the plume

- Portion of the column representing the source of the Electron Donor (Electron Donor) is initially filled with Electron Donor
- Remainder of the column is filled with Electron Acceptor (Electron Acceptor) to represent background concentration

What It Does

1D simulation progresses and dispersive mixing of Electron Donor and Electron Acceptor is followed by reaction

- Since column is transverse to plume only transverse dispersion is simulated
  - Advection and longitudinal dispersion are not simulated

What It Does

1D model results can be seen as a series of concentration profiles

- Simulation time of 1D model = travel time of a parcel of water leaving the plume source (*tt*)
- A steady, uniform velocity is assumed (*v*)
- Each concentration profile at time *tt* can be mapped to its location on the plume (*x*) using:

$$x = v.\ tt$$

Principal Assumptions

1. The source is continuous
2. Velocity field is steady and uniform
3. Reacting species travel at the same velocity, in the same parcel/column of water

   means that reactions with immobile (e.g. mineral) phases cannot be included

4. Longitudinal dispersion is unimportant in steady state plume

Inputs

Groundwater flow velocity

- Can also be calculated from K, I & n_e

Electron Acceptor background concentrations

- Electron acceptors (e.g. O_2, SO_4^{2-} etc.) in background groundwater

Electron Acceptor plume concentrations

- Electron acceptors (e.g. O_2, SO_4^{2-} etc) inside the plume

Inputs

Electron Donor background concentrations

- Electron donors (e.g. natural organic matter) in background groundwater

Electron Donor plume concentrations

- Electron donors (e.g. Benzene, Xylenol) inside the plume

Sensitive Parameters

Ratio of plume Electron Donor and background Electron Acceptor concentration

Plume velocity

- dispersion at the scale of diffusion
- limits application of model to low velocity plumes (for now)
  - less than ~ 2 cm/day

Analytical Model

Based on a closed form analytical solution to the advective-dispersive-reactive transport equation

- Simulates advection, dispersion and instantaneous biodegradation of a finite continuous source

Assumptions

1. An oxidisable contaminant will be degraded by bacteria
2. Bacteria degrade virtually instantaneously
3. Velocity is constant and uniform
4. Source is continuous

Inputs

Groundwater flow velocity

Transverse vertical dispersivity

- α_{TV}; can also be calculated from dz (thickness of the corona zone)
- α_{TH} and α_L commonly assumed to be 10 and 100 times α_{TV} (respectively)

Source width and thickness

Inputs

- Electron Acceptor background concentrations
- Electron Acceptor plume concentrations
- Electron Donor background concentrations
- Electron Donor plume concentrations

Outputs

- Plume Length
- Centreline Profile
- Vertical Profile
- Time to reach steady-state

Electron Balance Model

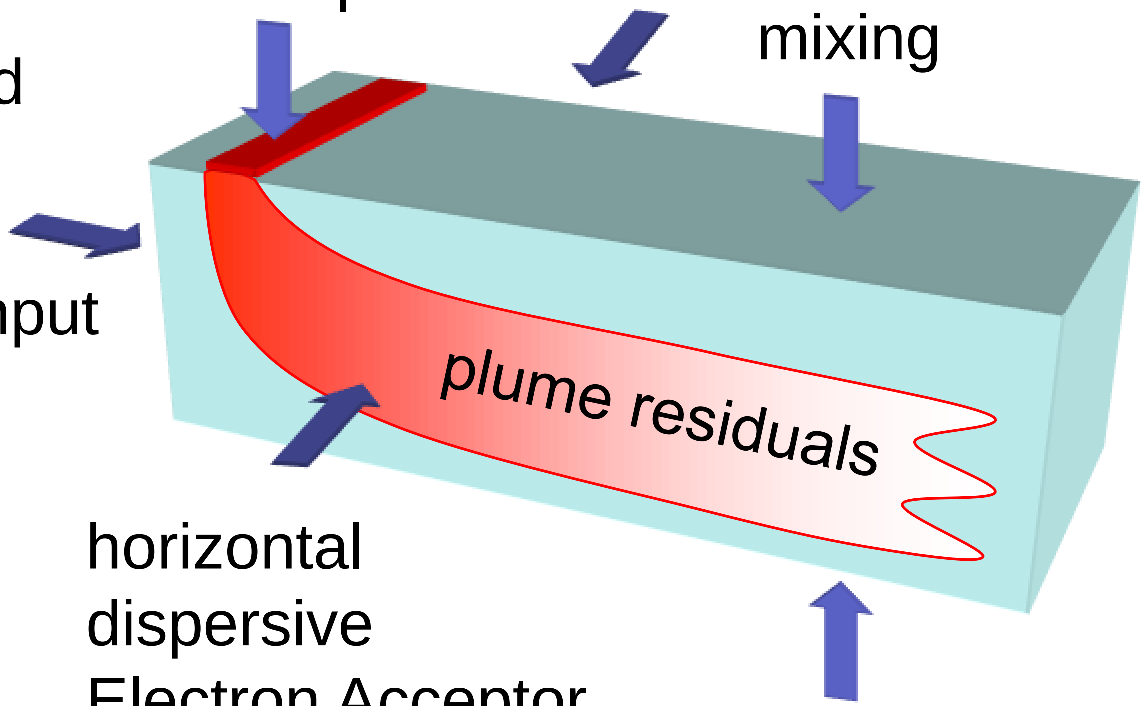
- Calculates inward dispersive mass flux of electron acceptors, and
- Mass flux (advective-dispersive) of electron donors away from the source
- Reacts Electron Donor with Electron Acceptor (instantaneous) until Electron Donor is zero

Schematic of EB model

source Electron
Donor input

vertical dispersive
Electron Acceptor
mixing

background
advective
Electron
Acceptor input



horizontal
dispersive
Electron Acceptor
mixing

What It Does

Calculates plume length

- iterates until Electron Acceptor and Electron Donor electrons are balanced
- plume length from velocity and time to balance electrons
- oxidisable contaminants only
- can account for fermentation and other core processes

Assumptions

1. An oxidisable contaminant will be degraded by bacteria
2. Bacteria degrade virtually instantaneously
3. Continuous source
4. Constant and uniform velocity

Inputs

Groundwater velocity

Vertical dispersivity

- horizontal dispersivity assumed 10x vertical

Plume width

Plume thickness

Mixing zone thickness

- thickness of reactive fringe in z direction
- or allow model to calculate from α_{TV}

Inputs

- Background Electron Acceptor concentrations
- Plume Electron Acceptor concentrations
- Background Electron Donor concentrations
- Plume Electron Donor concentrations
- Effective porosity
- Aquifer bulk density
- Fraction organic carbon

Outputs

Plume predictions

- Overall electron balance
- TOC flux at a given plume length
- maximum plume length
- Degradation rate constant

Time to reach steady-state

Carbon mass balance

What is the expected "resolution" for each model?

- Dependent on accuracy of key sensitive input parameters
- Effects of parameter variability on plume length differs for each parameter
  - some linear, some non-linear
- Most important parameter is α_{TV}
  - ability to resolve is limited

Děkuji za pozornost.