Risk Assessment of Contaminated Sites: From Source Zones to Water Resources

Vejle, Denmark 18-22 August

A System Dynamics Approach for the Integrative Assessment of Contaminated Land Management Options

Ursula S. McKnight, ursula.mcknight@uni-tuebingen.de
Michael Finkel, michael.finkel@uni-tuebingen.de
(University of Tübingen, Institute for Geoscience, Center for Applied Geoscience, Tübingen, Germany)

Motivation

- **Decreasing availability of land and water resources**
  - Undeveloped, uncontaminated land a scarce resource in today's Europe
  - Re-use of brownfields as accompanying strategy to reduce land consumption
  - Need for cost-effective assessment tools and methodologies

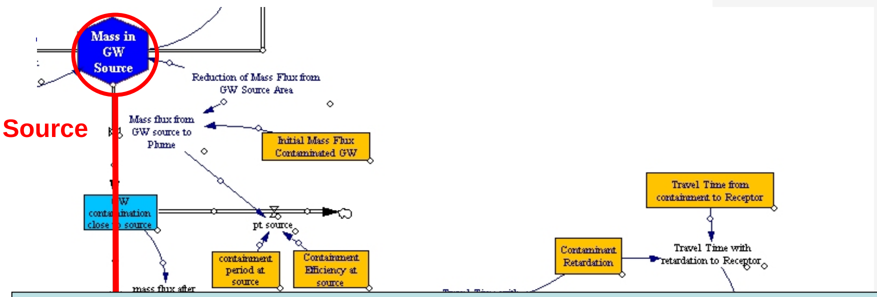
- **Implementation of novel approaches for brownfield redevelopment within German and EU law**
  - **Prerequisites:**
    - Pre-definition of verifiable objectives (space & time) → interim results (data)
    - Specification of monitoring measures
    - Development of (conventional) measures should NA prove inadequate
  - **Precautionary Principle:** applies to soil/GW protection → GW regarded as a receptor
  - **Principle of Proportionality** must be fulfilled → administrative decision; implies that any measure must be feasible (costs & efforts)

→KORA: implementing NA for contaminated land management (www.natural-attenuation.de)
→Helmholz Centre for Environmental Research (UFZ)

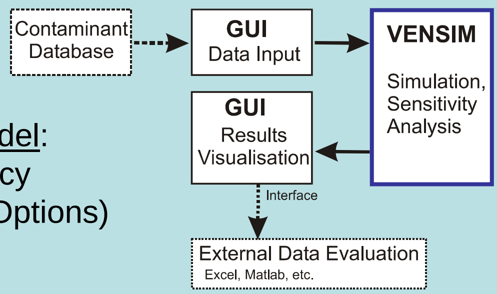
Preliminary assessment

- **Understand the problem: risk assessment & prediction**
  - Identify endangered receptors
  - Prioritization of management units (“hotspots”)
  - Improve conceptual site models
  - Support the implementation of risk-based methodolgies
- **Early consideration of management options**
  - Estimation of costs vs. Impacts over time
  - Pre-selection of suitable remediation strategies
- **Begin to answer relevant questions**
  - Source longevity
  - Future emission/mobility trends
- **Take uncertainty into account**
  - Identify critical parameters
  - Evaluate decision robustness
  - Improve efficiency of remediation projects

Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen
Eberhard Karls Universität Tübingen



- GUI-driven simulation model: *CARO-plus* (Cost-Efficiency Analysis of Remediation Options)



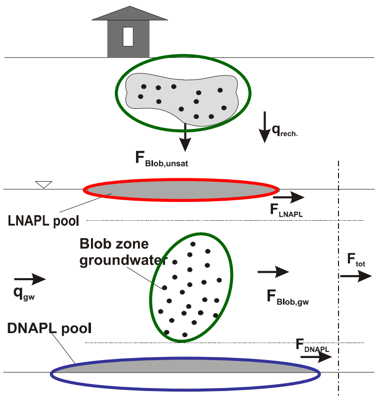
Center for Applied Geoscience (ZAG)

Research Center at the University of Tübingen

Eberhard Karls Universität Tübingen

Source: modeling the mass release

b) Raoult's law



$$C_{w,sat,i} = S_i * x_i * \gamma_i$$

LNAPL

Peter et al. (2007); Huntley and Beckett (2002)

$$F_i^{tot} = C_{w,i}^{sat} \cdot B_{NAPL} \cdot L_{NAPL} \cdot \left(q_{gwr} + \frac{T_{NAPL} \cdot \rho_r}{L_p} \cdot \bar{q} + \sqrt{\frac{4 \cdot D_{v,i} \cdot n_e \cdot q_{gw}}{\pi \cdot L_p}} + \frac{C_i^{a,sat} \cdot \bar{D}_{ea,i}}{C_i^{w,sat} \cdot z^{sur}} \right)$$

Blobs

$$L_{Blob} > L_{sat} \Rightarrow F_i^{Blob} = Q^{Blob} \cdot C_i^{w,sat} \qquad Q_{Blob} = \frac{v_a}{n_e} \cdot T_{NAPL} \cdot B_{NAPL}$$

$$L_{Blob} \le L_{sat} \Rightarrow F_i^{Blob} = Q^{Blob} \cdot C_i^{w,sat} \cdot e^{\left(\frac{-k \cdot T_{NAPL} \cdot B_{NAPL} \cdot L_{sat} \cdot n \cdot C_i^{w,sat}}{M_{Blob,i}} \cdot t \right)}$$

Grathwohl (1998)

DNAPL

$$F_i = 2 \cdot C_i^{w,sat} \cdot n \sqrt{\frac{D_i^w + \alpha_t \cdot v_a}{\pi \cdot \frac{L_{NAPL}}{v_a}}} \cdot L_{NAPL} \cdot B_{NAPL}$$

Eberhardt & Gratwohl (2002)

Center for Applied Geoscience (ZAG)

Research Center at the University of Tübingen

Eberhard Karls Universität Tübingen

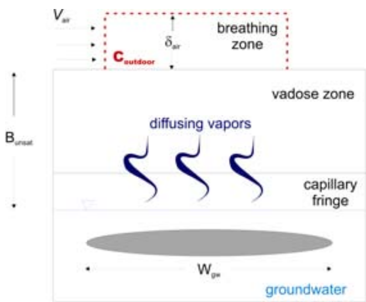
Risk assessment: groundwater

- Exposure pathway:

  Outdoor Air Inhalation

  – Physics-based models

  – Analyze pollutant behaviour in various media + transport through and between media



$$C_{outdoor} = C_{gw} * (H' / (1 + (U_a * da * L_{gw}) / (W_{gw} * D_{ws})))$$

$$D_{oai} = C_{outdoor} U_{di} F_{oi} * \frac{ED}{(BW * AT)}$$

$$HQ_i = \frac{D_{oai}}{RfD_i} ; RL_i = D_{oai} * SF_i$$

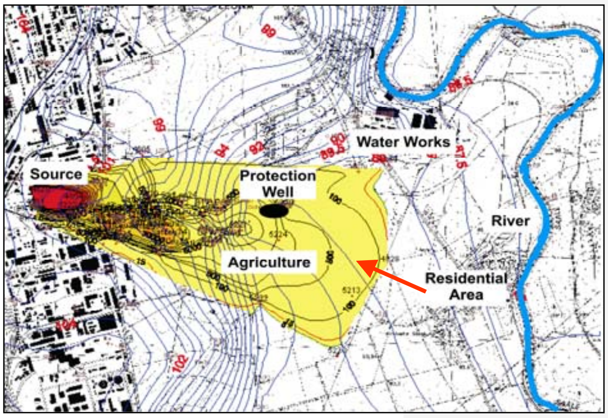
- **Risk modules for 15 exposure pathways → MEPAS** (Multimedia Environmental Pollutant Assessment System; Strenge & Smith (2006); ASTM (2002))

Case study: petroleum refinery

- Source zone:
  production buildings,
  storage tanks,
  loading docks

- COC: **MTBE** →
  potential for exposure
  to surface waters and
  residential areas

- 3 potential receptors identified
  - example results shown for potential **Residential Area expansion**



Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen
Eberhard Karls Universität Tübingen

Development of base case scenario

Exposure pathways	Maximum HQ_i [-]
Drinking water ingestion	**13.45**
Leafy vegetable ingestion	**10.21**
Soil ingestion	4.22E-06
Inhalation of re-suspended soil	9.85E-10
Outdoor air inhalation	2.75E-04
Indoor air inhalation	3.28E-05
Soil dermal contact	3.06E-06
Total maximum HQ_{tot} [-]	23.66

For *t* = 06-2006

Risk targets

$HQ_{tot} = 1$

RL_{tot} = 1E-5 (Germany)

Concentration target (LAWA, 2004)

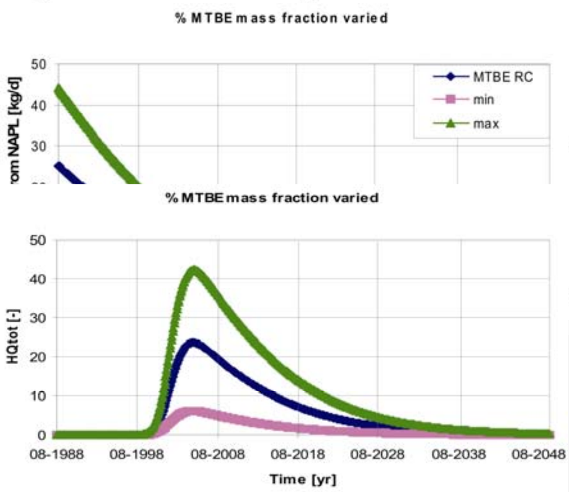
C_{mtbe} = 0.015 mg/L

Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen

Eberhard Karls Universität Tübingen

Deterministic results

- ➢ Quantitative impact assessment
- ➢ ID critical parameters
  - – ID data gaps
  - – ID uncertainties
- ➢ Multiple targets considered



Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen

Eberhard Karls Universität Tübingen

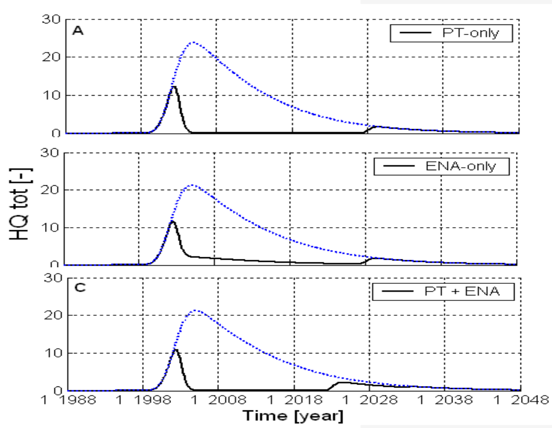
Assessment of technical measures

- ➢ Selected management options:

- P&T for 25 years
- Compare with ENA? *(for 8% MTBE)*

↓

- ➢ Enhancement = ?
  - 2.5x shown in Fig. B
  - 10x necessary for $HQ_{tot} = 1$



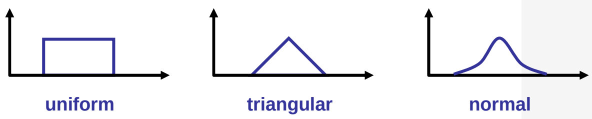
- ➢ Technology combinations if 10x not feasible
  - Optimization required for combined strategies !

Decision-making under uncertainty

- Site-specific parameters

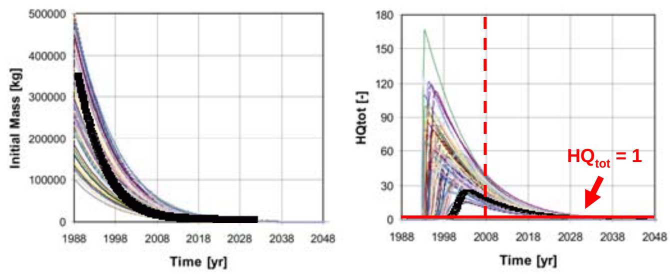
Parameter	Estimate	Distribution	Min	Max	Peak	StDev	Norm StDev
MTBE mass fraction [-]	0.08	Uniform	0.02	0.15		0.03	0.30
MTBE degradation rate GW [yr^{-1}]	0.28	Triangular	0.12	1.2	0.28	0.08	0.23
GW recharge rate [mm yr^{-1}]	40	Triangular	35	55	40	4.74	0.11
Hydraulic conductivity [m d^{-1}]	12.67	Triangular	12	42	12.67	7.65	0.32
Transverse vertical dispersivity [m]	0.0005	Uniform	0.0001	0.001		0.0002	0.46

Parameter Distributions



Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen
Eberhard Karls Universität Tübingen

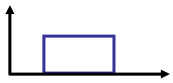
Probabilistic results



Decision-making under uncertainty

- Exposure parameters

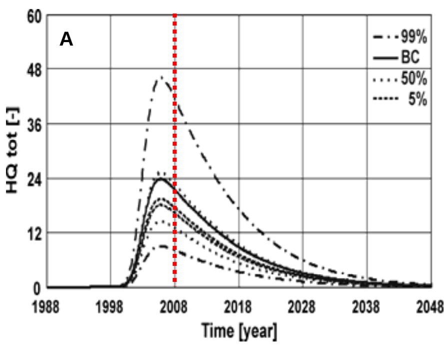
Parameter	Estimate	Min	Max	StDev	Norm StDev
Drinking water ingestion rate	2.0	1.0	3.0	0.58	0.29
Time fraction (# days for consumption)	1.0	0.25	1.0	0.22	0.35
Leafy vegetable ingestion rate	0.028	0.014	0.042	0.01	0.29
Time fraction (# days for consumption)	1.0	0.25	1.0	0.22	0.35
Translocation factor	1.0	0.25	1.0	0.22	0.35



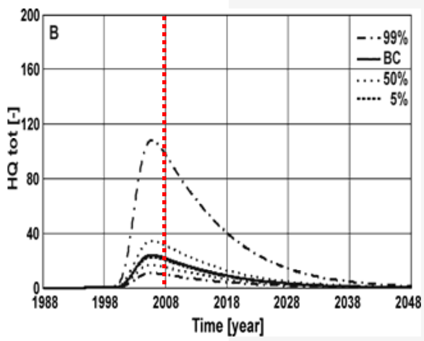
uniform

Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen
Eberhard Karls Universität Tübingen

Probabilistic results

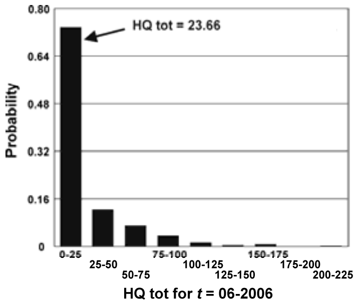


A) Drinking water ingestion pathway parameters

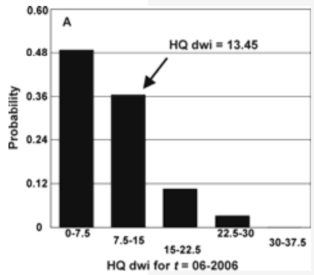


B) Leafy vegetable ingestion pathway parameters

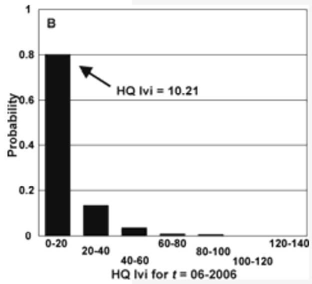
Probability distributions



➢ Site-specific properties



➢ Exposure properties



Center for Applied Geoscience (ZAG)
Research Center at the University of Tübingen
Eberhard Karls Universität Tübingen

Summary & Outlook

➢ **Preliminary Assessment & *CARO-plus***
- New approach based on system dynamics modeling
- Quickly screens cost-effectiveness/applicability of remediation strategies
- Streamlines the decision-making process
- Allows the prioritization of "hotspots"
- Higher abstraction level means higher uncertainties

➢ **Evaluate uncertainty**
- Sensitivity analyses include contaminant dependent/independent factors
- Best case — worst case/"what if" scenarios can be conducted
- Critical parameters can be identified

➢ **What's in the future:**
- Coupling to external models (e.g. Modflow, GIS) for catchment scale analysis
- Addition of new technologies (e.g. LNAPL phase extraction module)
- Optimization module

Questions ?

References:

ASTM (American Society for Testing and Materials), 2002. Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites. E1739-95, ASTM International, West Conshohocken, PA, USA.

Eberhardt, C. & Grathwohl, P., 2002. Time scales of organic contaminant dissolution from complex source zones: coal tar pools vs. blobs. *Journal of Contaminant Hydrology* 59, 45-66.

Huntley, D. & Beckett, G.D., 2002. Persistence of LNAPL sources: relationship between risk reduction and LNAPL recovery. *Journal of Contaminant Hydrology* 59, 3-26.

Grathwohl, P., 1998. Diffusion in Natural Porous Media: Contaminant Transport, Sorption/Desorption and Dissolution Kinetics. Springer-Verlag: New York, pp. 224.

Peter, A., Miles & B., Teutsch, G., 2007. Estimation of emission from an LNAPL contaminated zone considering groundwater recharge. *Environmental Geology*, DOI: 10.1007/s00254-007-0978-1.

Strenge, D.L. & Smith, M.A. 2006. Multimedia Environmental Pollutant Assessment System (MEPAS): Human Health Impact Module Description, Pacific Northwest National Laboratory (PNNL-16164), Prepared for the U.S. Department of Energy, Contract DE-AC06-76RLO 1830.