## Unit 6: Identification and assessment of pollution and uncertainties in groundwater modelling

Hans Peter Nachtnebel



### **Structure of the Presentation**

- Objectives
- Introduction and background
- Methodology
- Application
- Conclusion and results



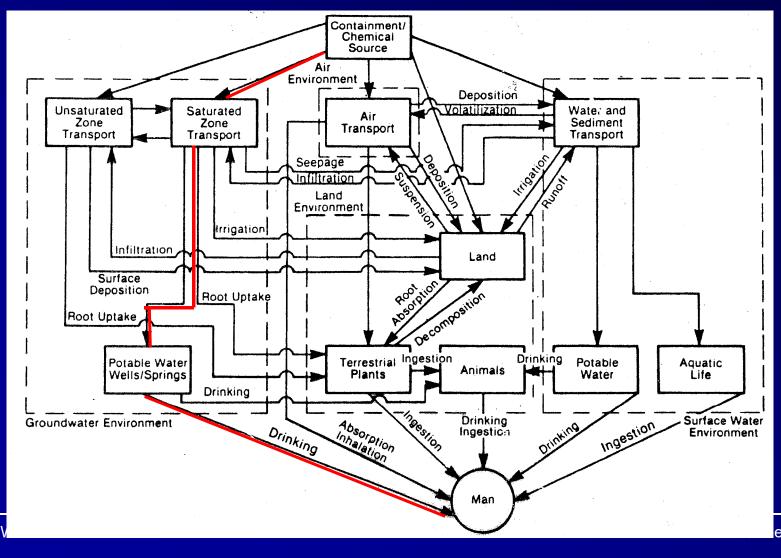
# **Objectives**

- A regional groundwater system suffers from nitrate pollution originating from different sources
- The groundwater system is used for regional drinking water supply
- The pollution sources have to be identified and the spatio-temporal variability of nitrate concentration has to be assessed to assist in water supply management

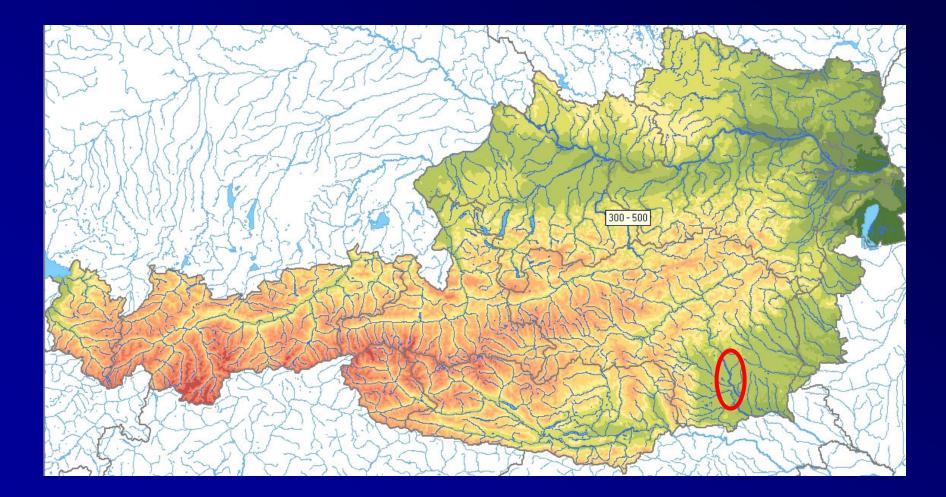




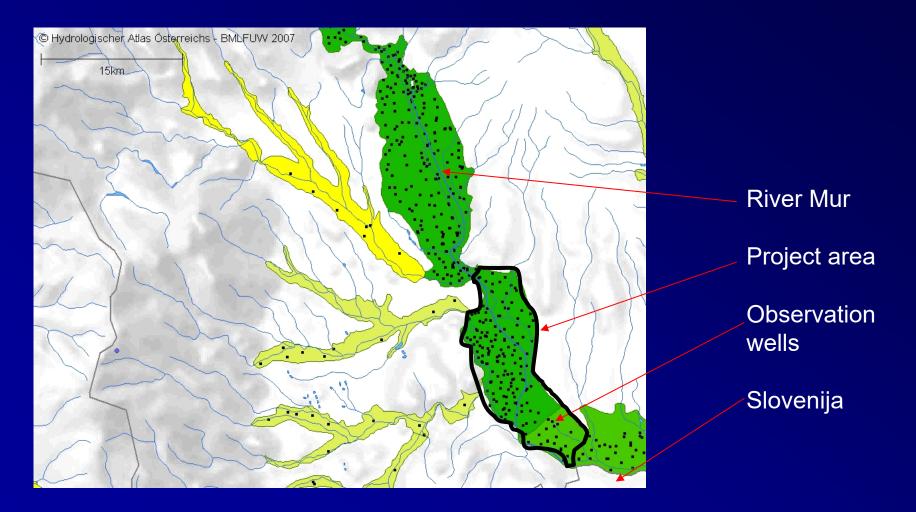
#### From Exposure to Dose: Environmental Transport Processes



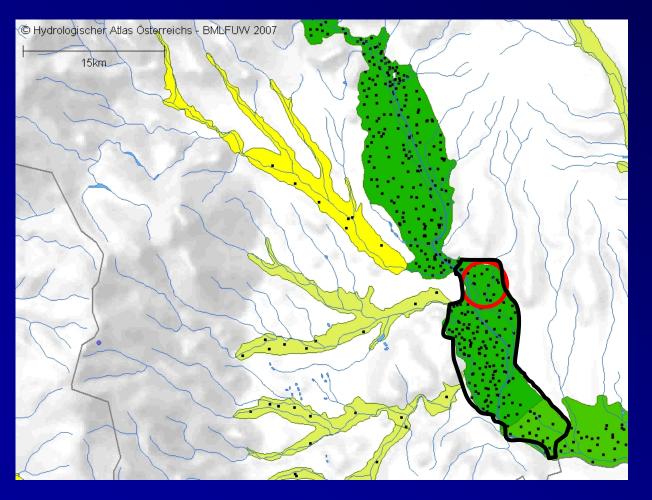
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#### **Detailed analysis**



- A shallow alluvial aquifer along the river Mur is utilized for regional drinking water supply
- Intensive agricultural land use (corn, lifestock farming) has led to a continuous increase in nitrate loads and subsequently to an increase of nitrate concentrations of the groundwater
- The concentrations show a large spatiotemporal variability and the water managers would like to improve their knowledge about peaks in nitrate concentration



## Tasks of the Study

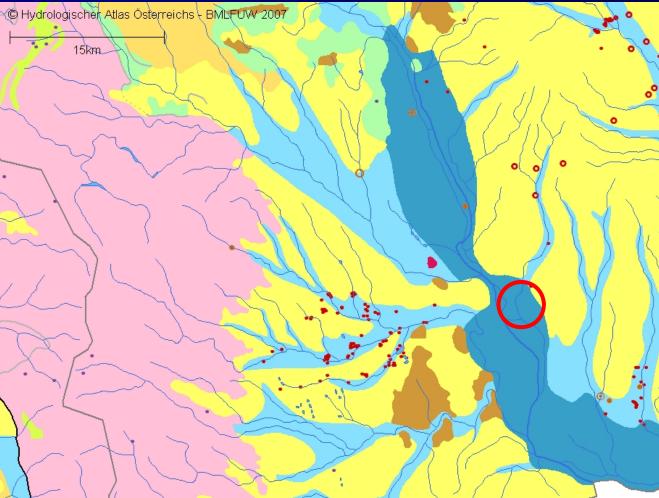
- Origin of pollutants
- Flow of pollutants
- Uncertainty in estimates of nitrate concentratrions

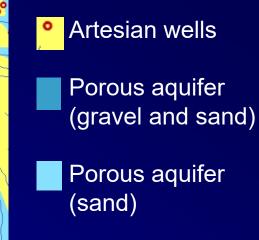


# **Available Data**



### Hydrogeology of the Groundwater System





Tertiary sediments (silt)

**GW Pollution Risk** 

H.P. Nachtnebel

### Land Use

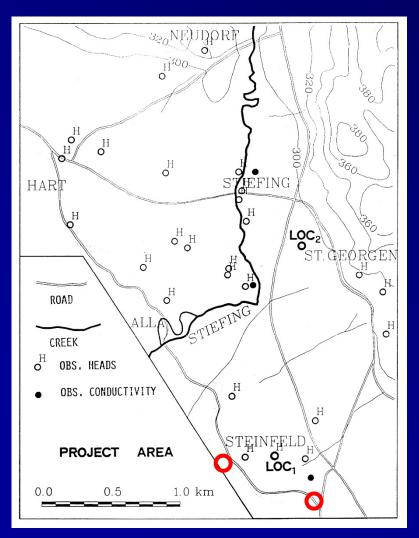




### **Data Base**

- Groundwater table is regularly monitored at 26 stations in a biweekly interval
- Groundwater quality at 22 locations monthly 195 sampling points within the initial campaign
- Hydrogeological data
   3 pumping test locations in the project area
   8 from outside but near by
   12 boreholes and geoelectric data
- Soil map, land use data

### **The Project Area**



2 of several water supply wells in the region



# Methodology

- Analysis of sampling data to identify sources •
- Geostatistical analysis of concentration data •





# Methodology

- Analysis of sampling data to identify sources
- Geostatistical analysis of concentration data
- Application of a 2D-solute transport groundwater model
   What could it help ?
   Which additional conclusions can be drawn ?

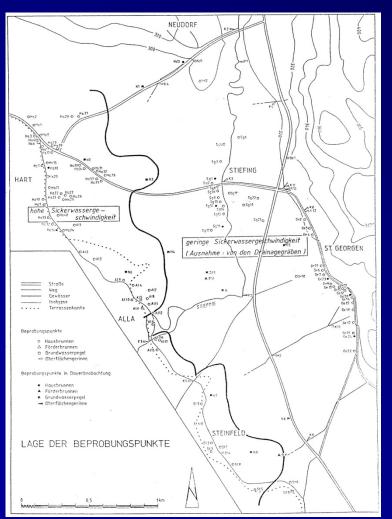


- The nitrate concentrations vary in time and space
- The sampling points are quite irregularly distributed over the region
- The nitrate concentrations show a trend from North to South
- An extension of kriging "External Drift Kriging" is applied





### **Detailed Monitoring Program**



Within a monitoring campaign about 105 wells were sampled

Irregularly distributed (clustering)

25 wells are regularly monitored

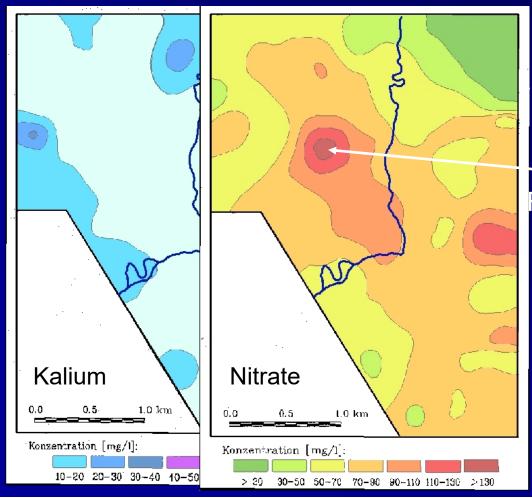


# Water Quality Monitoring

- Temperature
- Electrical conductivity
- NH4
- NO3-Nitrate
- NO2-Nitrite
- Phosphorous (diss., particulate, Ortho)
- **TOC**
- Diss. Oxygen
- Hardness of water
- Carbonate, Ca, K, Mg, .....



#### Some Results from the Monitoring Program



king Septic Tank or Sewer

#### Fertilizer and manure applicatior



- Nitrate data from first sampling campaign were statistically analysed
- Declustering (Journel, 1983) was applied due to irregular locations



$$\gamma^*(h) = \frac{1}{2n(h)} \cdot \sum W_{ij} \left( c(\underline{x}_i) - c(\underline{x}_j) \right)^2$$

$$h = I\underline{x}_{i} - \underline{x}_{j}I$$

$$W_{ij} = 1 \quad \text{for } h < 2 \text{ ho}$$

$$W_{ij} = \frac{1}{n_{i} \cdot n_{i}} \quad \text{else}$$

For small distances a regular variogram estimation For large distances an average is assumed



• Kriging is a BLUE estimator and it provides both

estimation of the expectation value

estimation of the uncertainty (estimation variance)

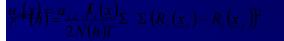


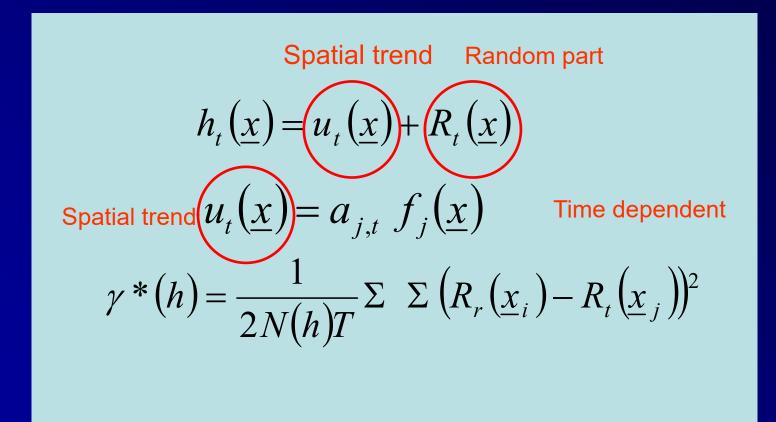


 The data set may exhibit a spatial trend Universal or External Drift Kriging

 The data set may exhibit spatio-temporal features

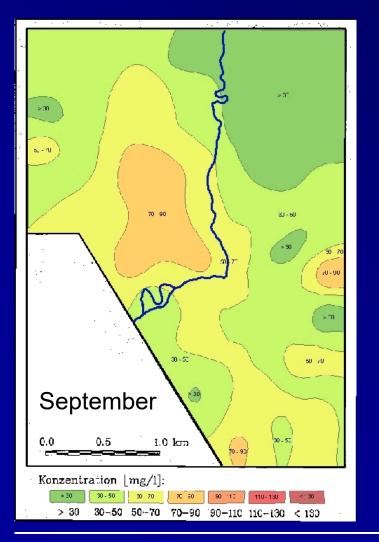


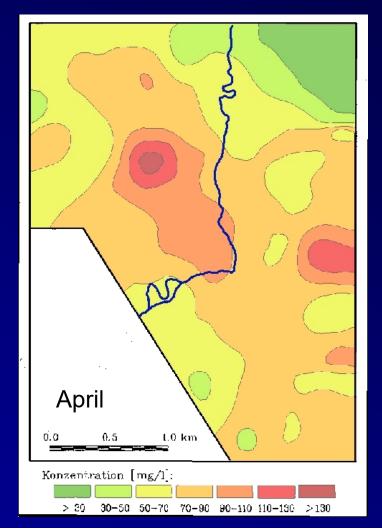






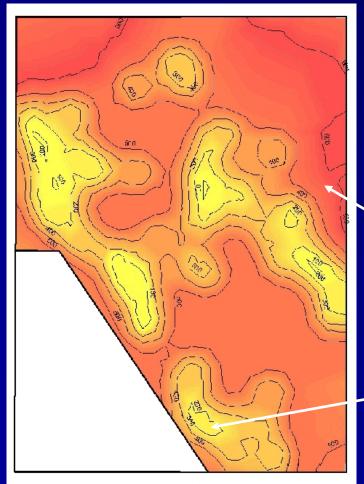
### **Spatial Distribution of Nitrate Concentration**







### **Results from Geostatistical Analysis**



ESTIMATION VARIANCE OF KRIGED NITRATE CONCENTRATION

High Uncertainty (22-26 mg/l)

Low Uncertainty (14 mg/l)



### **Conclusions from the Statistical Analysis**

- Pollution sources could be identified
- Nitrate pollution is highly variable in space and time
- The estimation uncertainty is very large

How could we improve our knowledge about the system ??



### Application of a 2D Solute Transport Groundwater Model

L. F. Konikow and J. D. Bredehoeft, "Computer Model of Two-Dimensional Solute Transport and Dispersion in Groundwater," Techniques of Water-Resources Investigations of the USGS; Chapter C2, Book 7, 1978, p. 90.

#### The Konikov-Bredehoeft model was used

Groundwater flow equation  

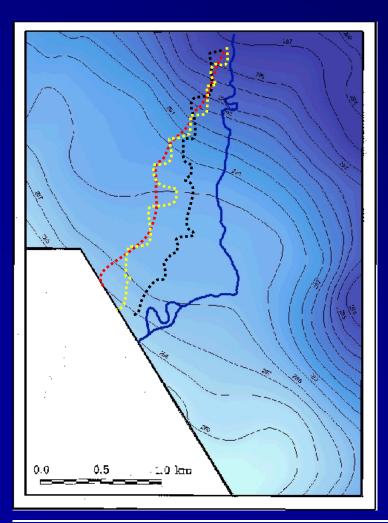
$$\frac{\partial}{\partial x_1} \left( bK_{11} \frac{\partial h}{\partial x_1} \right) + \frac{\partial}{\partial x_1} \left( bK_{12} \frac{\partial h}{\partial x_2} \right) + \frac{\partial}{\partial x_2} \left( bK_{21} \frac{\partial h}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( bK_{22} \frac{\partial h}{\partial x_2} \right) = S \frac{\partial h}{\partial t} + W(x_1, x_2, t)$$

$$\frac{\partial}{\partial x_1} \left( bD_{11} \frac{\partial C}{\partial x_1} \right) + \frac{\partial}{\partial x_1} \left( bD_{12} \frac{\partial C}{\partial x_2} \right) + \frac{\partial}{\partial x_2} \left( bD_{21} \frac{\partial C}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( bD_{22} \frac{\partial C}{\partial x_2} \right)$$
$$= \frac{\partial}{\partial x_1} \left( bCV_{x_1} \right) + \frac{\partial}{\partial x_2} \left( bCV_{x_2} \right) + \frac{\partial(Cb)}{\partial t} + \frac{C'W}{\epsilon}$$

Dispersion introduces additional uncertainty



### Flow and Dispersion



Groundwater flow (perpendicular to iso-lines)

Particle movement (yellow and black) (plus a random component)



### **Parameter Estimation**

 Based on the few local data plus from outside data variograms were estimated for hydraulic conductivity, bottom layer, heads (initial and boundary conditions)



### **Parameter Estimation**

 Based on the few local data plus from outside data variograms were estimated for hydraulic conductivity, bottom layer, heads (initial and boundary conditions)

Due to limited data there is a large uncertainty in these parameters



## **Model Calibration**

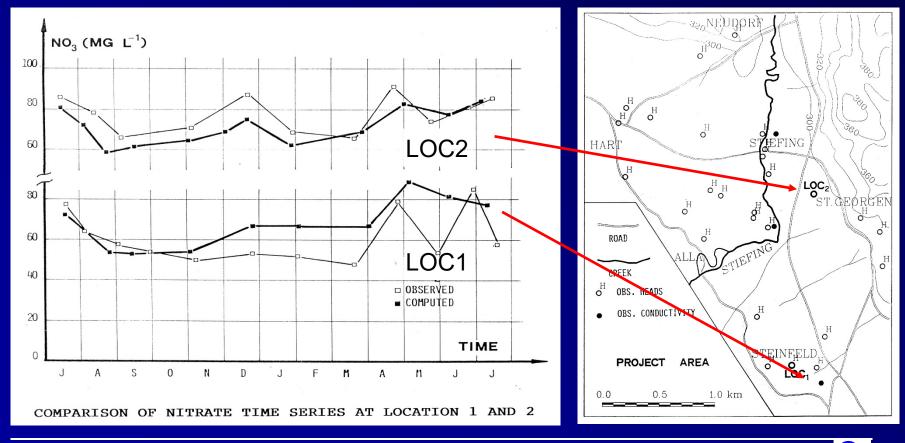
- Time series of heads and concentrations should be well reproduced
- The spatial pattern should be well reflected



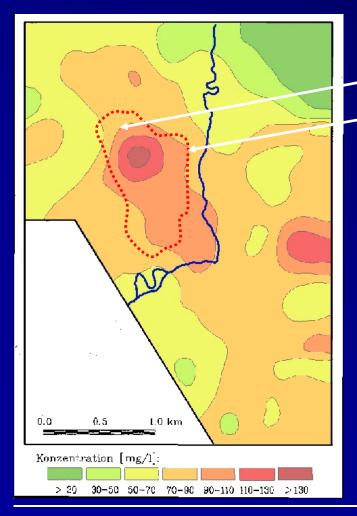


### **Model Calibration**

#### Observed heads and concentrations in time



#### Model Calibration with Respect to Pattern

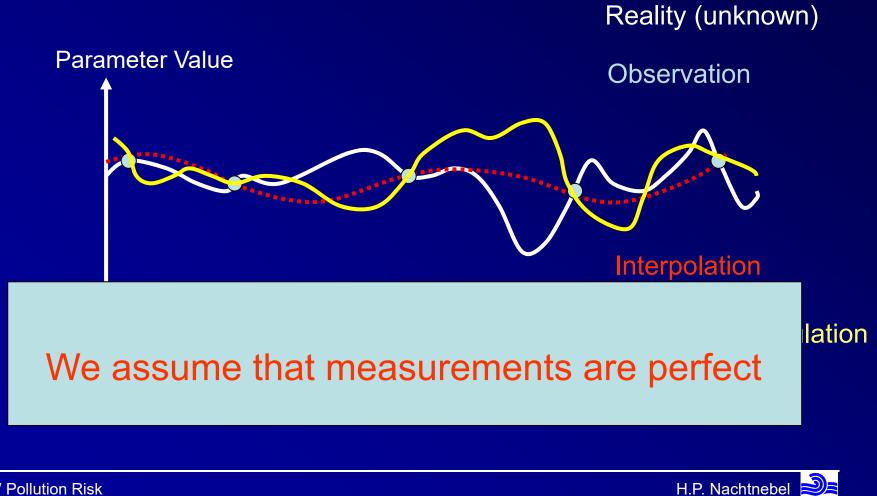


Contour lines of same concentration level From model From observation (interpolation)

Ratio of overlapping area to outside areas



### **Uncertainty in Model Parameters**



## **Conditional Simulation**

- Hundreds of different bottom layers, hydraulic conductivity fields, initial conditions are generated
- All of them have the same probability and fit the observations
- Each input results in a different GW model output (flow field and concentration pattern)

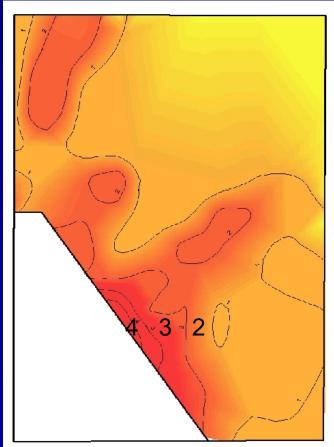


## **Results from Simulation**

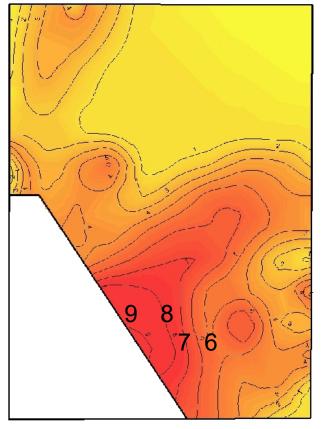
- For each grid point we get hundreds of NO3 time series
- We can estimate the uncertainty in the model output
- We can see the importance (significance) of an input parameter for the output (sensitivity)



### Estimation Uncertainty of Nitrate (mg/l)



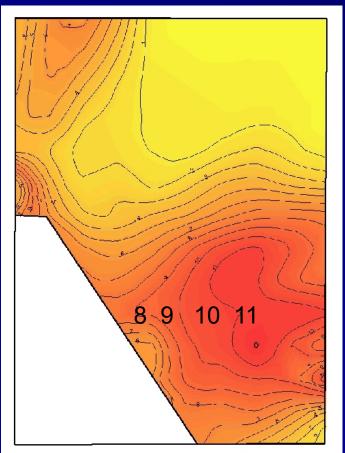
Estimation standard deviation Simulated saturated thickness



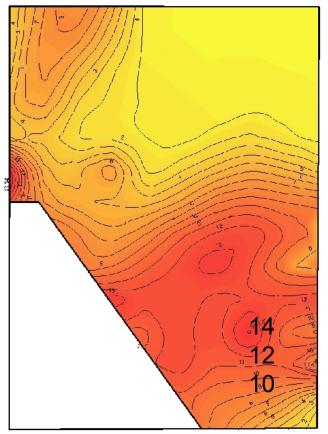
Estimation standard deviation Simulated K values



### Estimation Uncertainty of Nitrate (mg/l)



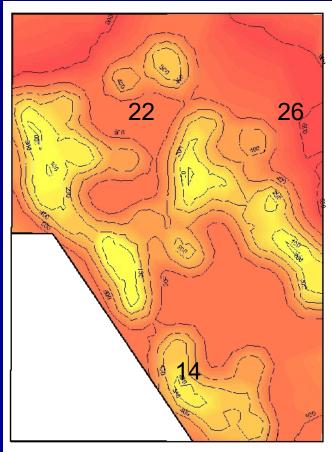
Estimation standard deviation Simulated boundary head values



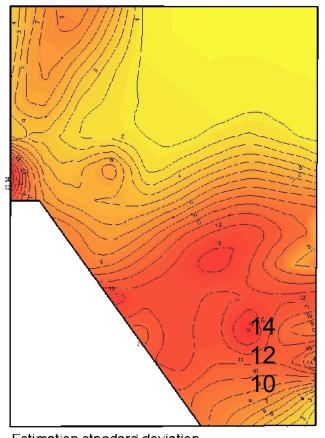
Estimation standard deviation Overall uncertainty



### **Comparison of Geostatistics with Model**



ESTIMATION VARIANCE OF KRIGED NITRATE CONCENTRATION



Estimation standard deviation Overall uncertainty





### Conclusions

- The overall uncertainty in Nitrate concentrations is larger in the geostatistical analysis than in the **GW-model** output
- Why? •





## Conclusions

- The overall uncertainty in Nitrate concentrations is larger in the geostatistical analysis than in the GW-model output
- Why ?
- We have included additional information (data and knowledge e.g. flow and transport model)





### Conclusions

- Here, heads (initial and boundary conditions) are the largest source of uncertainty
- Then hydraulic conductivity
- Bottom layer information is not so relevant



## Assesing the impacts

- Until now the probability of exceeding a pollution level has been estimated
- Possible consequences:
  - New wells have to be drilled
  - Water purification systems have to be developed
  - Water transfer from another region

**GW Pollution Risk** 

. . . . .



# Summary

- A groundwater pollution problem was analysed by geostatistical methods and by a physically based approach
- Estimates of pollution level as well as the respective uncertainties are available
- The incorporation of a model had reduced the overall uncertainty



# Thank you for your attention



