Modelling, monitoring and misinterpretation - the challenges of meaningful exposure assessments

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Pesticide Behaviour in Soils, Water and Air
27-29 March 2006
University of Warwick, UK

DuPont Crop Protection

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Key steps in exposure modelling

- Selection and/or modification of appropriate model
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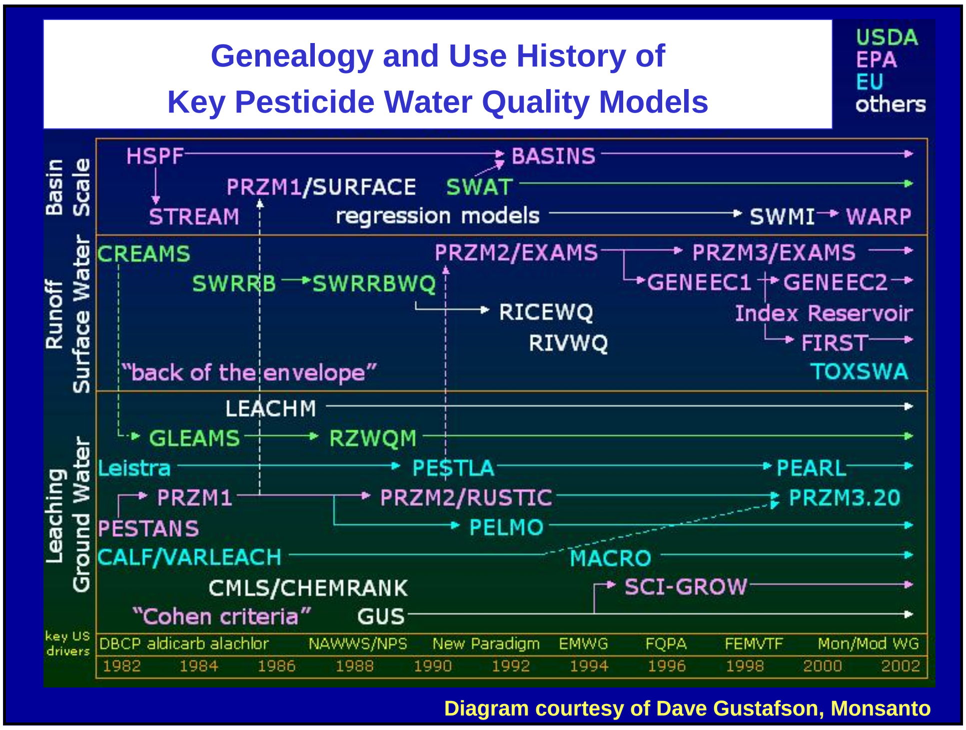
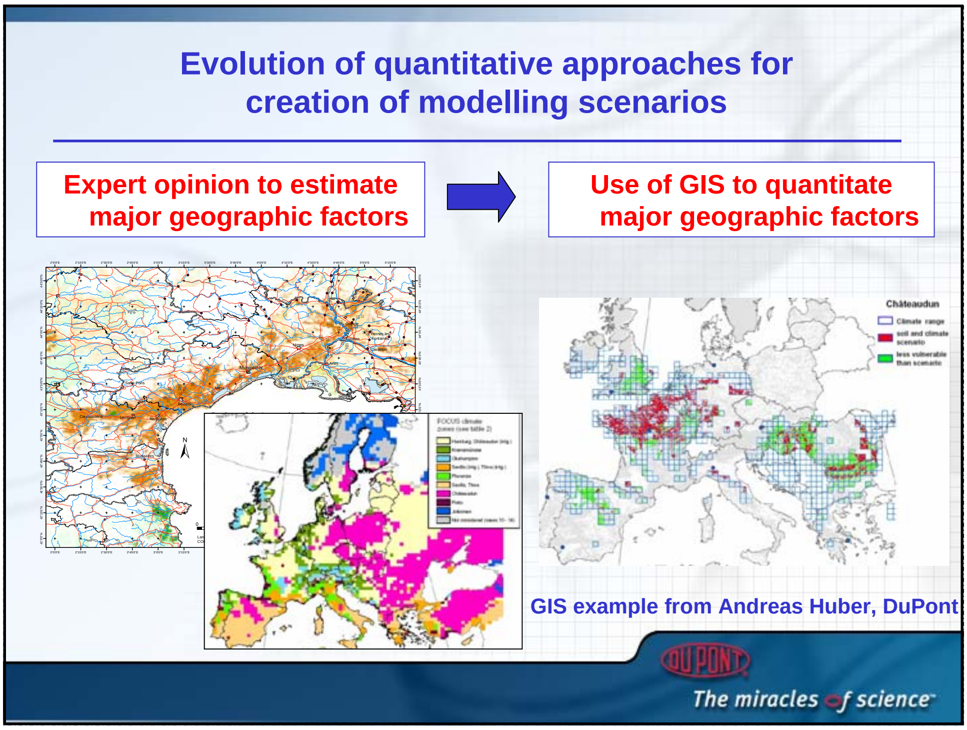

Genealogy and Use History of
Key Pesticide Water Quality Models
USDA
EPA
EU
others
Basin Scale
Runoff Surface Water
Leaching Ground Water
HSPF
BASINS
PRZM1/SURFACE
SWAT
STREAM
regression models
SWMI
WARP
CREAMS
PRZM2/EXAMS
PRZM3/EXAMS
SWRRB
SWRRBWQ
GENEEC1
GENEEC2
RICEWQ
Index Reservoir
RIVWQ
FIRST
"back of the envelope"
TOXSWA
LEACHM
GLEAMS
RZWQM
Leistra
PESTLA
PEARL
PRZM1
PRZM2/RUSTIC
PRZM3.20
PESTANS
PELMO
CALF/VARLEACH
MACRO
CMLS/CHEMRANK
SCI-GROW
"Cohen criteria"
GUS
key US drivers
DBCP aldicarb alachlor
NAWWS/NPS
New Paradigm
EMWG
FQPA
FEMVTF
Mon/Mod WG
1982
1984
1986
1988
1990
1992
1994
1996
1998
2000
2002
Diagram courtesy of Dave Gustafson, Monsanto


Evolution of quantitative approaches for
creation of modelling scenarios
Expert opinion to estimate
major geographic factors
Use of GIS to quantitate
major geographic factors
Châteaudun
GIS example from Andreas Huber, DuPont
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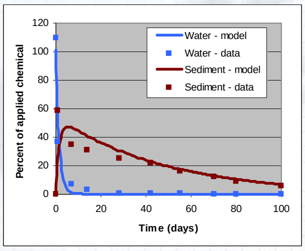
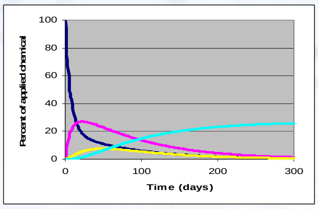
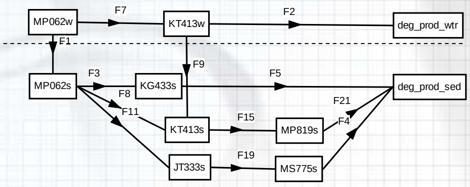
Approaches to selection of chemical e-fate data

Sources of environmental fate data

- taken from guideline GLP studies
- guidance on kinetic evaluations
- specific endpoints calculated
  - mean / median / geomean
  - specific percentile (80-90)
  - conservative / worst-case





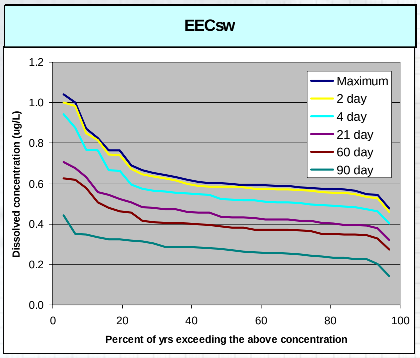


Approaches to selection of modelling results

Deterministic,
with a single set of inputs

PECsoil		
Time after last application (days)	Actual PECsoil (ug/kg)	TWA PECsoil (ug/kg)
0	269.0	--
1	263.7	266.4
2	258.5	263.7
4	248.3	258.5
7	233.8	251.0
14	203.1	234.5
28	153.3	205.8
50	98.5	169.7
100	36.1	116.0

Probabilistic,
with variation in one or more inputs



Regulatory

Key steps in exposure modelling

Fixed ☑

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  - Environmental fate (including metabolites)
  - Application data
- *Fixed* ☑ Calculation of model results
- *Fixed* ☑ Comparison with effects data to assess risk
- *Not required* Comparison with monitoring data

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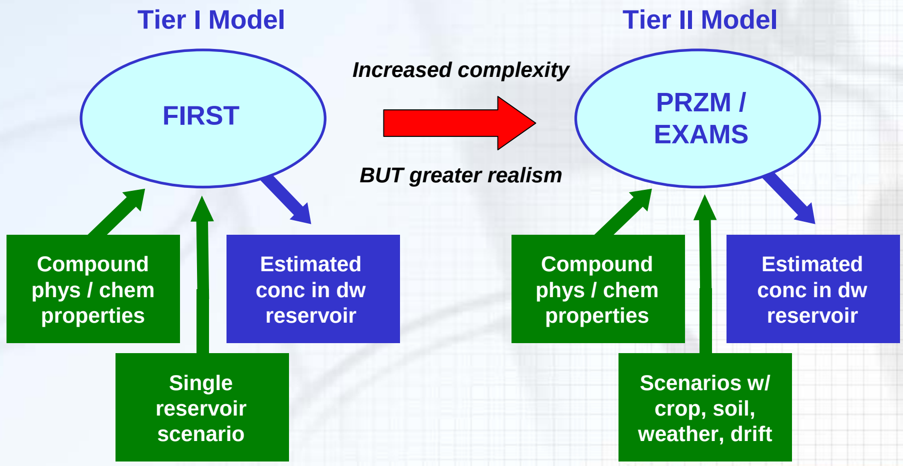
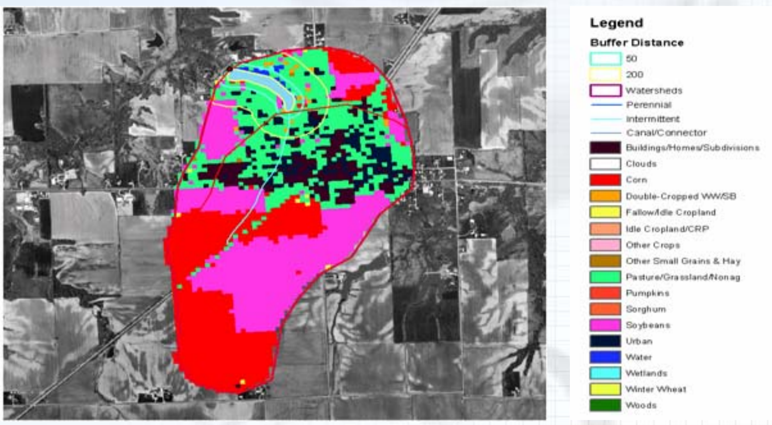
USEPA approach to modelling of surface water in drinking water reservoirs



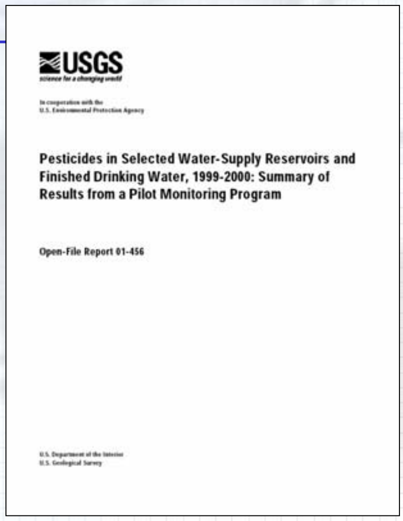
Conceptual Tier II drinking water reservoir



172.8 ha watershed drains into a 5.3 ha reservoir

Surface water monitoring data

- USGS data
- 12 drinking water reservoirs of various sizes in 12 states of USA
- 178 pesticides and degradation products
- Two years of sampling
- Weekly to quarterly sampling, with higher rate of sampling May to September



USGS

science for a changing world

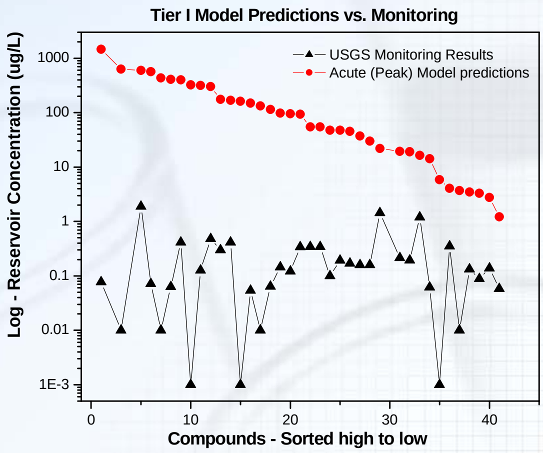
In cooperation with the U.S. Environmental Protection Agency

Pesticides in Selected Water-Supply Reservoirs and Finished Drinking Water, 1999-2000: Summary of Results from a Pilot Monitoring Program

Open-File Report 01-456

U.S. Department of the Interior
U.S. Geological Survey

Comparison of USEPA Tier I (FIRST) acute surface water modelling to monitoring



Maximum Measured Value from Study

Tier I modelling using FIRST is intended to be a screening evaluation of the potential to impact surface water quality

Comparison

- acute modelling results

- maximum monitoring data

(from highly vulnerable reservoirs with 11 to 37 samples per year)

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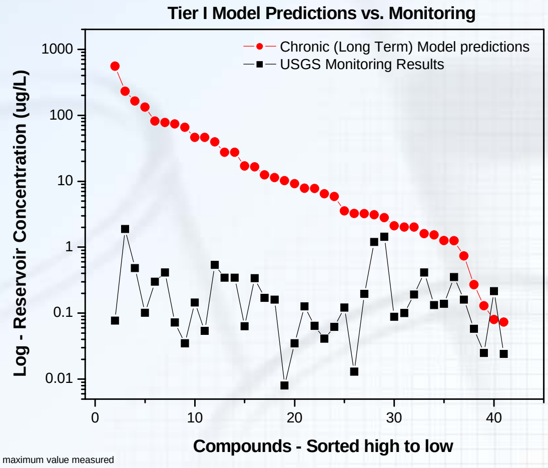
Comparison of USEPA Tier I (FIRST) chronic surface water modelling to monitoring



Used maximum value measured

Comparison

- chronic modelling results
- maximum monitoring data

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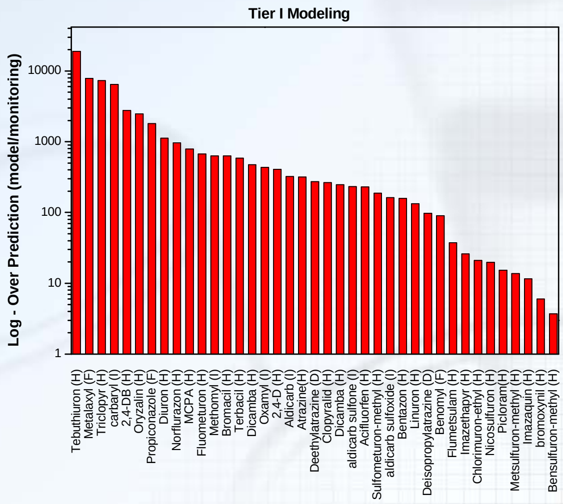
Extent of overprediction in USEPA Tier 1 acute modelling



Used Maximum Monitoring Value Found

Conclusion

Screening modelling using FIRST results in 1-4 orders of magnitude overprediction

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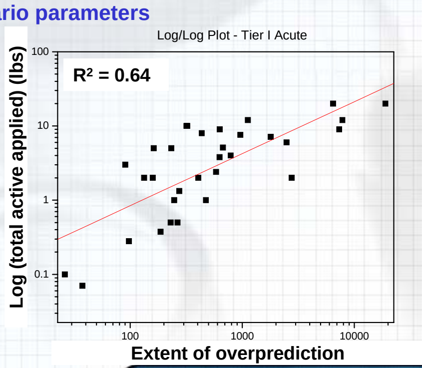
Factors contributing to overprediction of USEPA Tier 1 modelling

The <u>most significant factors</u> contributing to overprediction include:

- use of exaggerated chemical application rates in modelling
- use of conservative chemical property data (e.g. longest degradation half-lives)
- selection of worst-case / extreme scenario parameters

For FIRST modelling, the extent of overprediction was moderately correlated with the chemical use rate.



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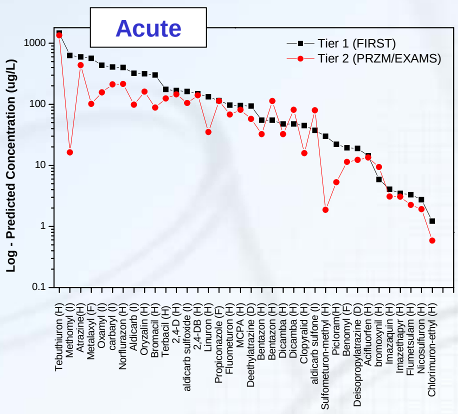
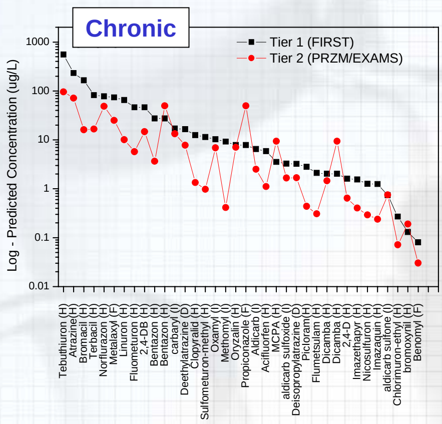
Exposure refinement obtained using USEPA Tier 2 (PRZM/EXAMS) modelling





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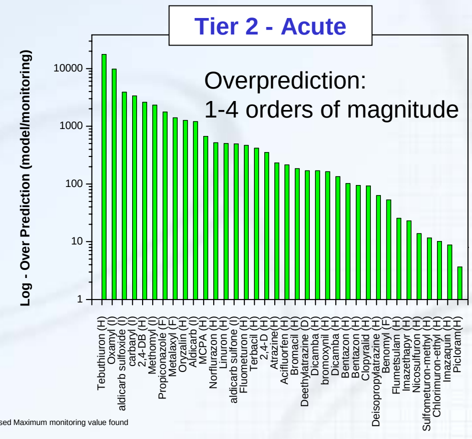
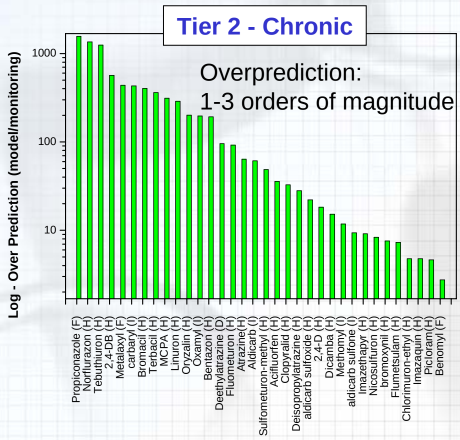
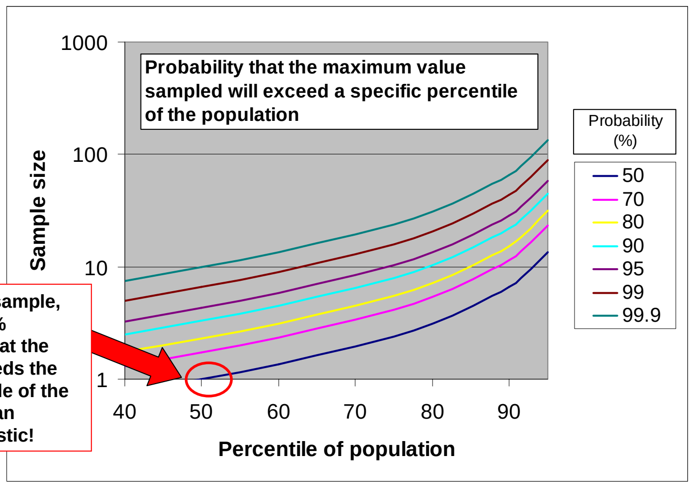
Overprediction obtained using USEPA Tier 2 (PRZM/EXAMS) modelling

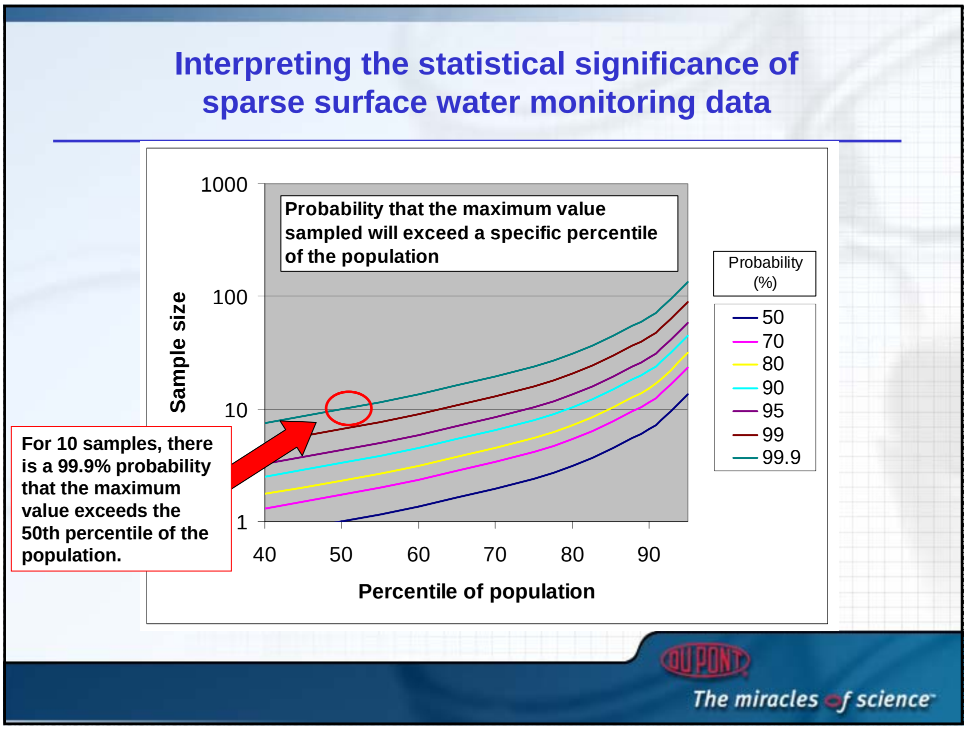




Interpreting the statistical significance of sparse surface water monitoring data



For a single sample, there is a 50% probability that the sample exceeds the 50th percentile of the population - an obvious statistic!


Interpreting the statistical significance of sparse surface water monitoring data
Probability that the maximum value sampled will exceed a specific percentile of the population
For 10 samples, there is a 99.9% probability that the maximum value exceeds the 50th percentile of the population.
Sample size
1000
100
10
1
40
50
60
70
80
90
Percentile of population
Probability (%)
50
70
80
90
95
99
99.9
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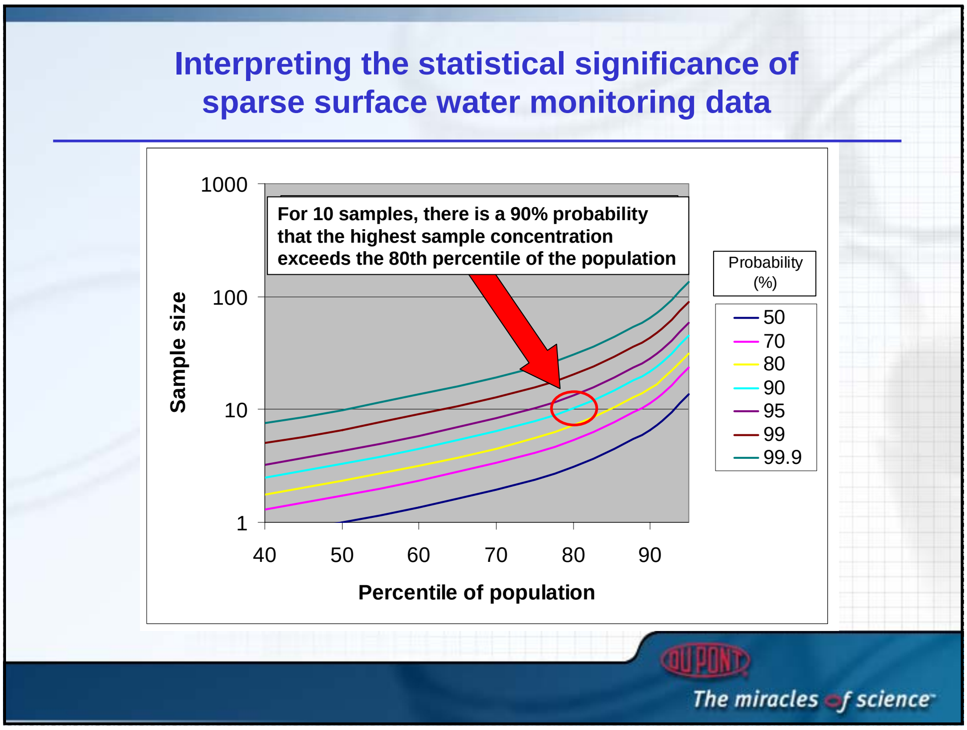
Interpreting the statistical significance of sparse surface water monitoring data
For 10 samples, there is a 90% probability that the highest sample concentration exceeds the 80th percentile of the population
Sample size
1000
100
10
1
40
50
60
70
80
90
Percentile of population
Probability (%)
50
70
80
90
95
99
99.9
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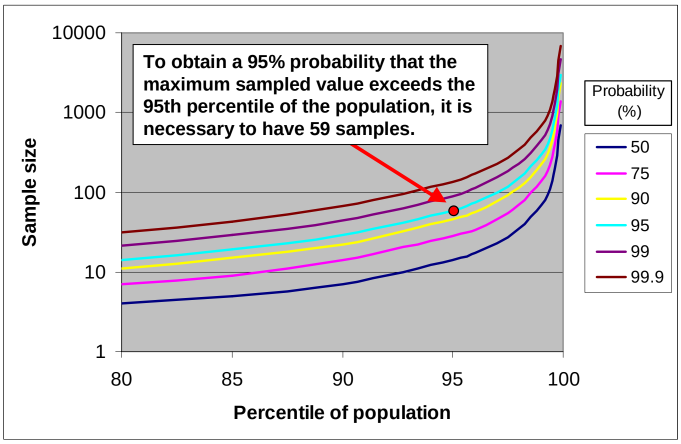
Interpreting the statistical significance of surface water monitoring data



ILSI, 1999. A Framework for Estimating Pesticide Concentrations in Drinking Water for Aggregate Exposure Assessments

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Experimental study of sampling frequency in a large drinking water reservoir

Annual sampling frequency	Percentile of annual mean atrazine concentration (ug/L)					
	50	75	90	95	99	Maximum
4	1.684	3.040	--	--	--	3.437
12	1.691	3.102	3.408	3.536	--	3.566
24	1.703	3.138	3.390	3.501	--	3.636
48	1.712	3.171	3.385	3.493	--	3.715
120	1.715	3.170	3.382	3.480	3.665	3.775
365	1.720	3.170	3.379	3.475	3.640	3.790

Data source: USGS Open-File Report 01-456

Conclusion: In this case, quarterly sampling is adequate for determining concentration distributions in drinking water reservoirs

Lower sampling frequencies may provide useful results when the distributions are stable and narrow

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Recommendations to improve interpretation of surface water modelling

- Typically, an unknown degree of conservatism is incorporated into regulatory model simulations as a result of:

  - use of fixed input data (scenarios, e-fate, appln data)
  - reporting of selected modelling results

- To help determine the extent of conservatism, it is appropriate to:
  - determine key factors contributing to predicted concentrations - e.g. drift values, hydrology, buffer width
  - evaluate the magnitude, duration and return frequency of critical value exceedence
  - compare regulatory modelling results with available monitoring data and evaluate possible reasons for differences

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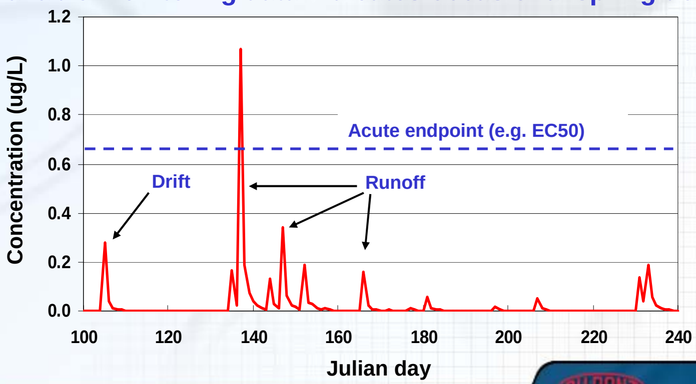
Analysis of key factors and exceedence frequency

- Primary issue in this case: runoff due to late spring rain events
- Exceedence appears to be a single event and can be reduced by controlling runoff
- Available monitoring data indicates occasional spring detections



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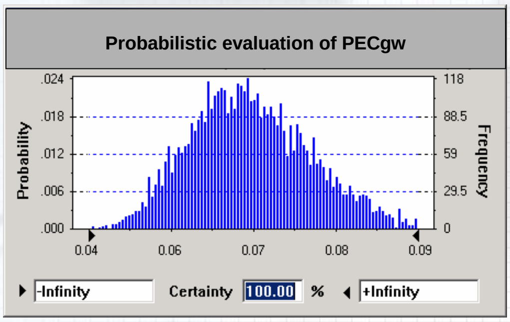
Higher tier developments in modelling: a groundwater example

- To support higher tier evaluations, it can be useful to express results probabilistically using distributions of key inputs such as chemical properties, time, location, etc.

Percentile	PECgw (ug/L)
0	0.04
10	0.06
20	0.06
30	0.06
40	0.07
50	0.07
60	0.07
70	0.07
80	0.08
90	0.08
100	0.11



Challenges in development of future surface water modelling

- Improved simulation of potential concentrations in small water bodies may require:
  - better representation of ditch, pond and stream hydrology
  - more realistic water body loading rates
  - a broader range of environmental scenarios
- Simulation of potential concentrations in surface water used as drinking water supplies may require:
  - development and use of watershed-scale models
  - evaluation of chemical use intensity within a watershed
- Finished drinking water concentrations can be impacted by:
  - mixing of source waters
  - filtration and carbon treatment
  - effects of chlorination / ozonation

Acknowledgments

- The coauthors of the work included in this presentation:

  Scott Jackson, BASF

  Paul Hendley, Syngenta

  Russell Jones, Bayer

  Nick Poletika, Dow

  Dave Gustafson, Monsanto

- Thank you for your attention!