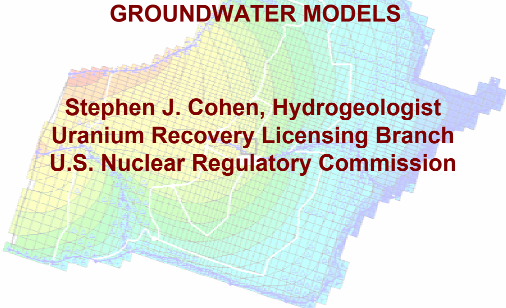
QUANTIFYING UNCERTAINTY IN GROUNDWATER MODELS



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WHY AM I TALKING ABOUT THIS?

TO DEMONSTRATE THAT UNCERTAINTY IN ANY TYPE OF MODEL COULD BE QUANTIFIED AND QUANTIFYING UNCERTAINTY CAN BE USEFUL TO BOTH THE REGULATORS AND THE REGULATED.

CONVEY AN UNDERSTANDING OF ONE METHOD OF QUANTIFYING MODEL UNCERTAINTY.

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DISCUSSION TOPICS

- REASONS FOR QUANTIFYING MODEL UNCERTAINTY
- DESCRIPTION OF THE MAXIMUM LIKELIHOOD BAYESIAN MODEL AVERAGING (MLBMA) METHODOLOGY
- RESULTS OF MLBMA
- EXAMPLE OF MLBMA

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WHY QUANTIFY MODEL UNCERTAINTY

- A THEORY HAS ONLY THE ALTERNATIVE OF BEING RIGHT OR WRONG. A MODEL HAS A THIRD POSSIBILITY; IT MAY RIGHT, BUT IRRELEVANT (Manfred Eigen, 1973).
- A MODEL BASED ON THE PRACTITIONER'S BEST GUEST IS INHERENTLY BIASED (Shlomo Neuman, 2006).
- QUANTIFYING UNCERTAINTY PROVIDES INFORMATION REGARDING THE DEGREE OF IRRELEVANCE, AND IT MINIMIZES BIAS.
- THIS DOES NOT REPRESENT A NEW REQUIREMENT!!!!

UNCERTAINTY ESTIMATION METHOD

- MAXIMUM LIKELIHOOD BAYESIAN MODEL AVERAGING (MLBMA).
- BASED ON PROCEDURES BY PNL, DRI-LAS VEGAS, UNIVERSITY OF ARIZONA (MEYER, P., YE, M., ROCKHOLD, M., CANTRELL, K., NEUMAN, S.)
- INCORPORATES MODEL, PARAMETER, AND SCENARIO UNCERTAINTY.
- CURRENT PAPERS AND GUIDANCE:
  - NUREG/CR – 6805
  - NUREG/CR – 6843
  - "ON EVALUATION OF RECHARGE MODEL UNCERTAINTY (MING YE, 2006)
  - "INFORMATION MATRIX" (JAY MYUNG AND DANIEL NAVARRO, 2004).

MLBMA METHOD

- BRIEF DISCUSSION OF BAYESIAN STATISTICS

BAYES' THEOREM

$$p(M_k \mid D) = \frac{p(D \mid M_k)\, p(M_k)}{\sum_{l=1}^{K} p(D \mid M_l)\, p(M_l)}$$

where:

$p(M_k \mid D)$ = posterior probability

$p(D \mid M_k)$ = likelihood of model M_k

$p(M_k)$ = prior probability

MLBMA METHOD (cont'd.)

- DEVELOP MODELS BASED ON REASONABLE ALTERNATIVES.
- JOINT CALIBRATION USING PEST.
- DETERMINE PRIOR PROBABILITIES.
- CALCULATE INFORMATION CRITERION AND RANK MODELS.
- CALCULATE POSTERIOR PROBABILITIES
- PERFORM MONTE CARLO SIMULATIONS FOR PARAMETER UNCERTAINTY FOR EACH MODEL.
- COMPUTE PROBABILITY DENSITY FUNCTIONS (PDFs) FOR EACH MODEL.
- COMPUTE EXPECTATION (MEAN OF DISTRIBUTION), VARIANCE, AND MODEL AVERAGED PDF.

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MLBMA METHOD

- END RESULTS

EXPECTATION
$$E[\Delta \mid D] = \sum_{i=1}^{K} E[\Delta \mid D, M_k] p(M_k \mid D)$$

VARIANCE
$$Var[\Delta \mid D] = \sum_{i=1}^{K} Var[\Delta \mid D, M_k] p(M_k \mid D) + \sum_{i=1}^{K} (E[\Delta \mid D, M_k] - E[\Delta \mid D])^2 p(M_k \mid D)$$

MODEL-AVERAGED PDF
$$p(\Delta \mid D) = \sum_{k=1}^{K} p(\Delta \mid M_k, D) p(M_k \mid D)$$

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MLBMA METHOD

- END RESULTS

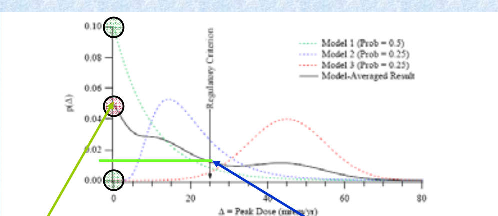

Figure 1-5. Model averaged probability density function for the three-model example of Figure 1-4 with model probabilities (see legend) used as weights

(Meyer, P.D., et al.)

0.1*0.5 + 0*0.25 + 0*0.25 = 0.05
.009*0.5 + .0270*0.25 + .005*0.25 = 0.0125

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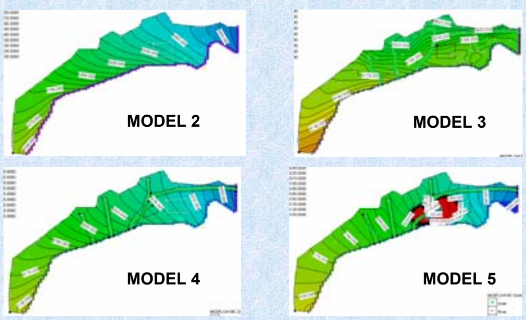
MODEL DEVELOPMENT

- MODELS DEVELOPED USING GROUNDWATER MODELING SYSTEM (GMS).
- MODEL 2: AVERAGE VALUES FOR HYDRAULIC CONDUCTIVITY (HC), RECHARGE, AND EVAPOTRANSPIRATION (ET).
- MODEL 3: AVERAGE VALUES FOR HC AND ET, ZONE VALUES FOR RECHARGE.
- MODEL 4: AVERAGE VALUE FOR HC, ZONE VALUES FOR RECHARGE AND ET.
- MODEL 5: SAME AS MODEL 4 WITH A GENERAL HEAD BOUNDARY, RECHARGE, AND ET.

MODEL DEVELOPMENT (cont'd.)



MODEL DEVELOPMENT (cont'd.)

- BOUND MODEL SELECTION FROM THE SIMPLEST TO THE MOST REASONABLY COMPLEX.
  - MODEL ABSTRACTION – PROCESS OF MAKING COMPLICATED MODELS SIMPLE.
  - SIMPLE MODELS MORE EASILY CALIBRATED AND TEND TO BE MORE ACCURATE.
  - COMPLEXITY DOES NOT NECESSARILY TRANSLATE TO MORE ACCURACY, BUT WILL CERTAINLY INCREASE RUN TIMES.
- MLBMA PENALIZES COMPLEX MODELS.

JOINT CALIBRATION (cont'd.)

- CALIBRATE MODELS TO FIND OPTIMAL PARAMETERS.
- USE PEST WITH LOG TRANSFORMATION FOR HYDRAULIC CONDUCTIVITY.
- AFTERWARDS, IN "PARAMETERS" DIALOG BOX, INSERT OPTIMAL PARAMETERS AND UNCHECK "LOG TRANSFORM".
- SET NOPTMAX TO -1. THIS WILL GIVE YOU THE MATRICES YOU NEED FOR RANKING COMPUTATIONS.

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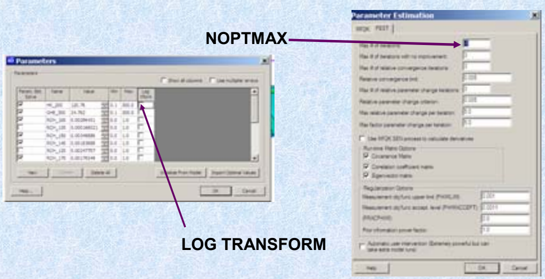
JOINT CALIBRATION (cont'd.)



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PRIOR PROBABILITY

- ESTIMATE BY MODELER OF THE CONFIDENCE HE/SHE HAS IN EACH MODEL (SUBJECTIVE).
- COMMON METHOD IS EXPERT ELICITATION
- PRIOR PROBABILITY BECOMES LESS IMPORTANT WITH MORE DATA

$$p(M_k \mid D) = \frac{p(D \mid M_k)\,p(M_k)}{\sum_{l=1}^{K} p(D \mid M_l)\,p(M_l)}$$

where:

$p(M_k \mid D)$ = posterior probability

$p(D \mid M_k)$ = likelihood of model M_k

$p(M_k)$ = prior probability

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PRIOR PROBABILITY (cont'd.)

PRIOR PROBABILITIES FOR THIS EXAMPLE

- MODEL 2 – 0.35
- MODEL 3 – 0.3
- MODEL 4 – 0.2
- MODEL 5 – 0.15

LIKELIHOOD

- USE DATA FROM JOINT CALIBRATION TO CALCULATE LIKELIHOOD
- NEED TO OBTAIN THE MAXIMUM LIKELIHOOD PARAMETER ESTIMATES TO CALCULATE NEGATIVE LOG LIKELIHOOD (NLL) AND FISHER INFORMATION MATRIX.
- DATA FOR NLL AND FISHER INFORMATION MATRIX IS FOUND IN THE .REC FILE THAT IS WRITTEN AFTER PEST RUNS.
- NLL = OBJECTIVE FUNCTION = WSSR

MODEL RANKING WITH KIC

- RANKING ACCOMPLISHED BY CALCULATING KASHYAP'S INFORMATION CRITERION (KIC)
- INFORMATION CRITERION PROVIDES AN INSIGHT INTO THE AMOUNT OF INFORMATION ONE CAN OBTAIN FROM A SET OF DATA.
- FISHER INFORMATION DEFINED AS THE COVARIANCE OF THE FIRST PARTIAL DERIVATIVES OF THE LOG-LIKELIHOOD.
- OTHER CRITERION AVAILABLE – AIC, BIC. KIC CONSIDERED BEST FOR GROUNDWATER APPLICATIONS.

MODEL RANKING WITH KIC (cont'd.)

$$KIC = N \ln \hat{\sigma}_{ML}^2 - N_k \ln 2\Pi + \ln|\mathrm{I}|$$

where:

$\ln|\mathrm{I}|$ = natural log of the determinant of the Fisher Information Matrix

$$\ln|\mathrm{I}| = -N_k \ln\left(\frac{N - N_k}{N}\right) - \sum_{i=1}^{N_k} \ln \lambda_i$$

$$\hat{\sigma}_{ML}^2 = \frac{WSSR}{N - N_k}$$

$WSSR =$ **Sum of the squared weighted residuals (WSSR) = NLL = objective function**

$N =$ **Number of calibration data**

$N_k =$ **Number of calibration parameters**

$\lambda_i =$ **Eigenvalues from .rec file**

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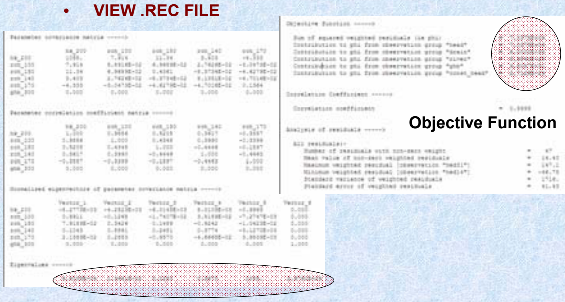
MODEL RANKING WITH KIC (cont'd.)

- VIEW .REC FILE



Objective Function

Eigenvalues

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MODEL RANKING WITH KIC (cont'd.)

- EXAMPLE KIC CALCULATION

Model 4			
Eigenvalues (Gamma)	ln Gamma	Nk =	9
2.96E-04	-8.12441	N =	44
3.18E-03	-5.75245		
1.35E-02	-4.30425		
1.36E-01	-1.99584		
1.90E-01	-1.66284		
2.34E-01	-1.45115		
5.57E-01	-0.58537		
1.15E+00	0.1415		
1.10E+02	4.695925		
	-19.0389		
Log of Fisher Determ	21.09845		
KIC	249.7247		

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MODEL RANKING WITH KIC (cont'd.)

- MODEL RANKS

Data	Model 2	Model 3	Model 4	Model 5
N	35	44	44	4.7000E+01
Nk	4	4	9	6.0000E+00
WSSR	8351	8023	1.16E+04	7.0375E+04
Sigma Square	238.6	182.3409091	262.9545455	1497.340426
ln|I|	14.19146623	14.78390375	21.0984541	-59.21097424
KIC	198.4575558	236.4910302	249.7247327	273.3997143

MOST LIKELY MODEL

POSTERIOR PROBABILITY

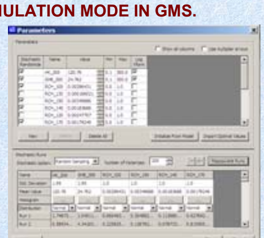
$$p(M_k \mid D) = \frac{\exp\left(-\frac{1}{2}\Delta KIC_k\right)p(M_k)}{\sum_{l=1}^{K}\exp\left(-\frac{1}{2}\Delta KIC_l\right)p(M_l)}$$

ΔKIC = lowest KIC subtracted from KICs for other individual models. ΔKIC for lowest model = 0.0

Data	Model 2	Model 3	Model 4	Model 5	
N	35	44	44	4.7000E+01	
Nk	4	4	9	6.0000E+00	
WSSR	8351	8023	1.16E+04	7.0375E+04	
Sigma Square	238.6	182.3409091	262.9545455	1497.340426	
ln|I|	14.19146623	14.78390375	21.0984541	-59.21097424	
KIC	198.4575558	236.4910302	249.7247327	273.3997143	
p(Mk) (Prior Probability)	0.35	0.3	0.2	0.15	1
p(Mk|D) (Posterior Prob)	0.999999995	4.72269E-09	4.21149E-12	2.28318E-17	1

PARAMETER UNCERTAINTY

- MONTE CARLO SIMULATIONS
- GENERATE RANDOM PARAMETERS AND COMPUTE SOLUTIONS FOR EACH MODEL BEING CONSIDERED
- USE STOCHASTIC SIMULATION MODE IN GMS.



PARAMETER UNCERTAINTY (cont'd.)

- FOR Δ (i.e. HEAD AT A WELL, CONCENTRATION AT A WELL) OF CONCERN, TABULATE RESULTS AND COMPUTE PROBABILITY DISTRIBUTION FUNCTION (PDF).
- COMPUTE MODEL EXPECTATION (MEAN OF PDF) AND VARIANCE.
- COMPUTE MODEL-AVERAGED PDF.
- THESE ARE YOUR FINAL ANSWERS.

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PARAMETER UNCERTAINTY (cont'd.)

- Δ = HEAD AT A PARTICULAR WELL
- PDF COMPUTED USING HISTOGRAM ANALYSIS
- EXPECTATION AND VARIANCE COMPUTED FOR EACH MODEL
- MODEL EXPECTATION AND VARIANCE (PREDICTIVE UNCERTAINTY COMPUTED FOR OVERALL MODEL
- MODEL-AVERAGED PDF CALCULATED

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PARAMETER UNCERTAINTY (cont'd.)

- PDF, EXPECTATION, AND VARIANCE COMPUTED FOR EACH MODEL

Bin	*Frequency*	Probability	Expect	Var
5200	4	0.08	416	3595.52
5400	39	0.78	4212	112.32
5600	7	0.14	784	4948.16
More	0			
Expectation			**5412**	
Variance				**8656**

EXPECTATION FOR MODEL 2

$$E[\Delta \mid D] = \sum_{k=1}^{K} E[\Delta \mid D, M_k] p(M_k \mid D)$$

TOTAL MODEL EXPECTATION

Posterior Mean	E	p(Mk|D)	E*p(Mk|D)
Model 2	5412	0.999999995	5411.999974
Model 3	5400	4.72269E-09	2.55025E-05
Model 4	5636	4.21149E-12	2.3736E-08
Model 5	5832	2.28318E-17	1.33155E-13
Sum - Total E			**5412.0**

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PARAMETER UNCERTAINTY (cont'd.)

- **POSTERIOR VARIANCE**

Posterior Variance	VAR	p(Mk|D)	VAR*p(Mk|D)	E	E-Total E ^2	p(Mk|D)	Product
(aka Predictive Uncertainty)							
Model 2	8656	0.999999995	8655.999959	5412.0	0	0.999999995	0
Model 3	0	4.72269E-09	0	5400	144	4.7227E-09	6.8007E-07
Model 4	305104	4.21149E-12	1.28494E-06	5636	50176	4.2115E-12	2.1132E-07
Model 5	1299776	2.28318E-17	2.96762E-11	5832	176400	2.2832E-17	4.0275E-12
			8655.99996				8.9139E-07
Total Predictive Uncertainty			**8655.999961**				
Total Standard Deviation			**93.03762659**				

$$Var[\Delta \mid D] = \sum_{i=1}^{K} Var[\Delta \mid D, M_k] p(M_k \mid D) + \sum_{i=1}^{K} (E[\Delta \mid D, M_k] - E[\Delta \mid D])^2 p(M_k \mid D)$$

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MODEL-AVERAGED PDF

- **PROBABILITY OF EACH RESPECTIVE BIN VALUE MULTIPLIED BY THE RESPECTIVE POSTERIOR PROBABILITY.**

$$p(\Delta \mid D) = \sum_{k=1}^{K} p(\Delta \mid M_k, D) p(M_k \mid D)$$

where:

$p(\Delta \mid M_k, D)$ = probability of Δ given a particular model and data set (i.e., bin value)

- **SUM ALL THE PRODUCTS AND PLOT.**

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MODEL-AVERAGED PDF (cont'd.)

					Weighted Probability				
Bin	Model 2	Model 3	Model 4	Model 5	Model 2	Model 3	Model 4	Model 5	**Average**
5200	0.08	0	0	0	0.08	0	0	0	**0.08**
5400	0.78	1	0.7	0.64	0.78	4.72E-09	2.95E-12	1.46E-17	**0.78**
5600	0.14	0	0.14	0.16	0.14	0	5.9E-13	3.65E-18	**0.14**
5800	0	0	0.04	0.04	0	0	1.68E-13	9.13E-19	**1.68E-13**
6000	0	0	0.02	0.02	0	0	8.42E-14	4.57E-19	**8.42E-14**
6200	0	0	0	0.02	0	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	0.02	0	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	0	0	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	0	0	0	8.42E-14	0	**8.42E-14**
7000	0	0	0.04	0	0	0	1.68E-13	0	**1.68E-13**
7200	0	0	0.02	0.02	0	0	8.42E-14	4.57E-19	**8.42E-14**
7400	0	0	0	0.02	0	0	0	4.57E-19	**4.57E-19**
7600	0	0	0	0.02	0	0	0	4.57E-19	**4.57E-19**
7800	0	0	0	0	0	0	0	0	**0**
8000	0	0	0.02	0	0	0	8.42E-14	0	**8.42E-14**
8200	0	0	0	0	0	0	0	0	**0**
8400	0	0	0	0	0	0	0	0	**0**

PROBABILITY OF 5200 OCCURRING IN MODEL 2 MULTIPLIED BY THE MODEL 2 POSTERIOR PROBABILITY

SUM OF ALL PRODUCTS FOR THE 5200 VALUE

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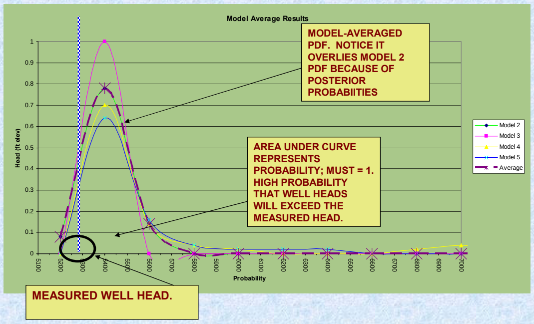
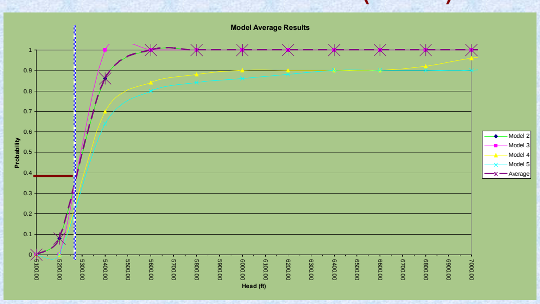
MODEL-AVERAGED PDF (cont'd.)

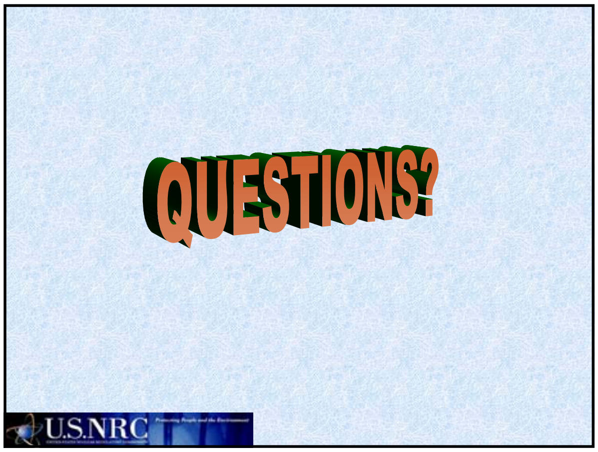


MODEL-AVERAGED PDF (cont'd.)



SUMMARY

- MLBMA PROVIDES A METHOD OF QUANTIFYING UNCERTAINTY.
- VALUABLE IN ASSESSING RISKS.
- CAN EXPEDITE REVIEWS BECAUSE MULTIPLE MODELS ARE EVALUATED.
- MLBMA CAN ALSO INCORPORATE SCENARIO UNCERTAINTY – NOT ADDRESSED IN THIS PRESENTATION.
- USEFUL IN OTHER TECHNICAL DISCIPLINES


QUESTIONS?
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