The findings and conclusions in this presentation are those of the author and do not necessarily represent the views of the Agency for Toxic Substances and Disease Registry or the U.S. Department of Health and Human Services

Hadnot Point, Camp Lejeune, NC

Reconstruction of Historical Contaminant Concentrations: A Computational Method

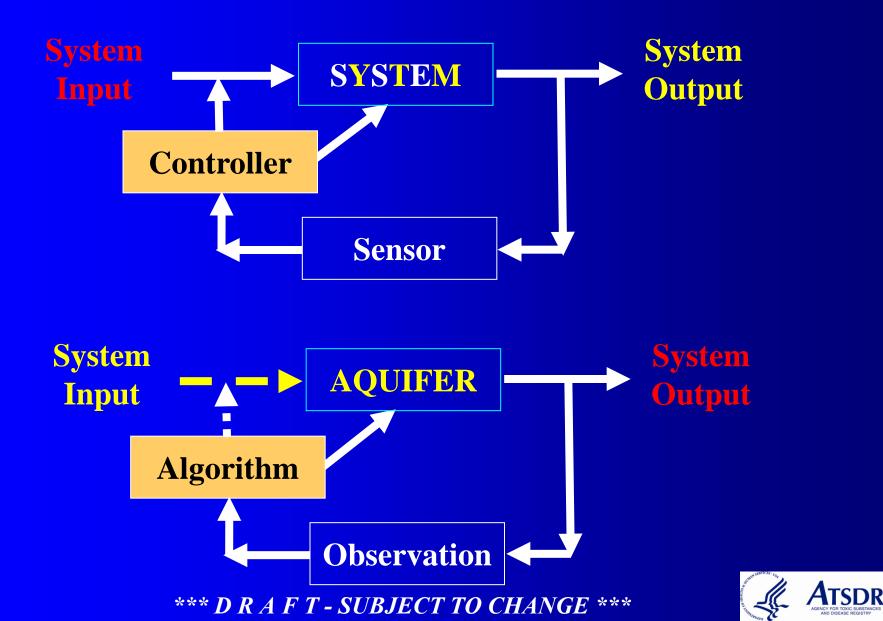
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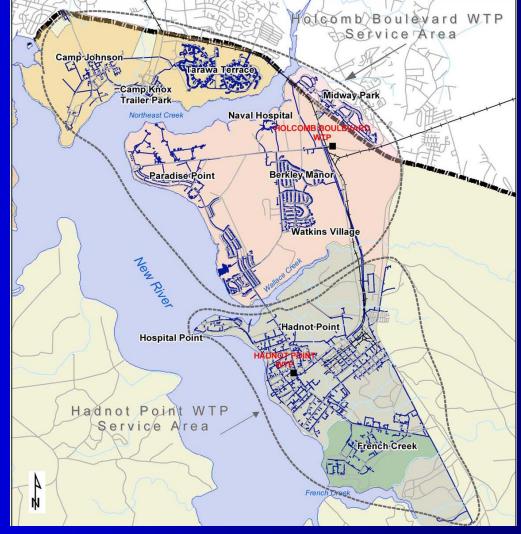


Control Theory Based Time Series Analysis



Camp Lejeune, NC Site:

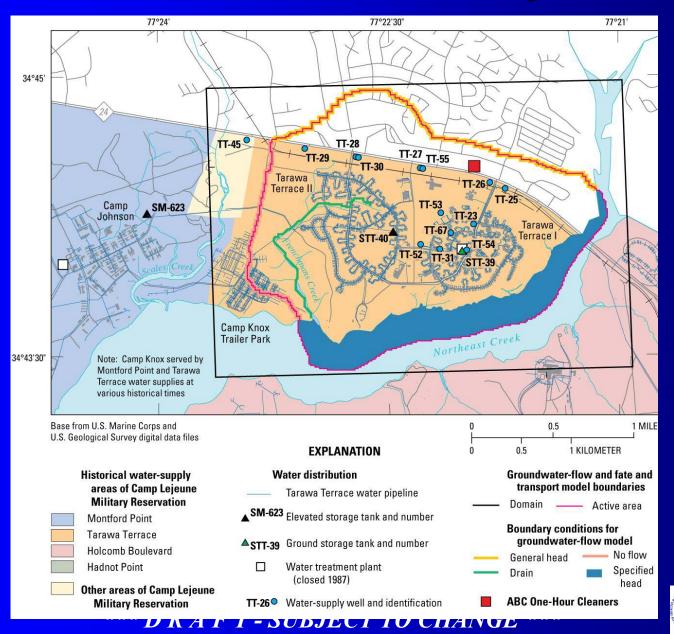








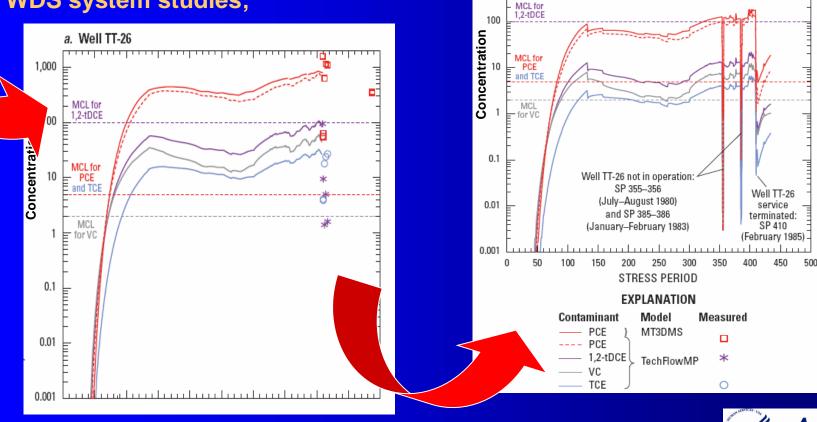
Tarawa Terrace Study:





Tarawa Terrace Study:

- Site data collection;
- Groundwater flow and contaminant fate and transport modeling;
 - Mixing model; and,
- WDS system studies;



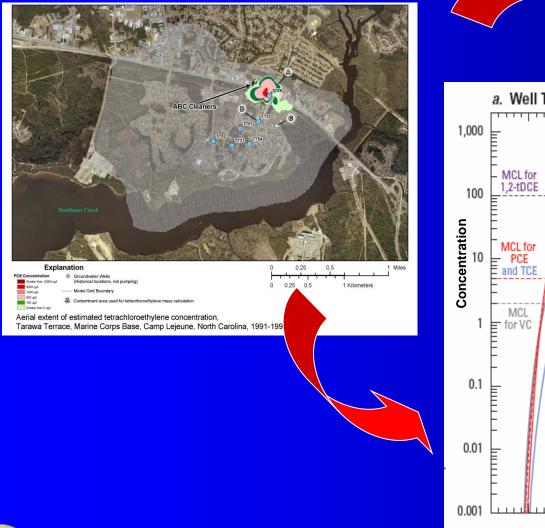
*** D R A F T - SUBJECT TO CHANGE

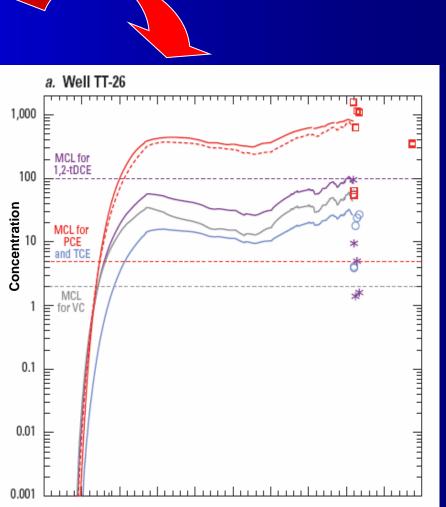
b. Water treatment plant (finished water)

1,000



The Purpose of the current study:









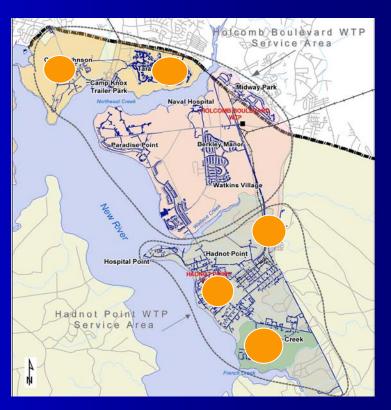
Starting Point and Expectations:

 The proposed method will be a screening level procedure;

 The proposed method is to be used locally (Source, GW Hyd. and fate);

• The accuracy expected from the model is a function of the quality and quantity of the data available at the locale;

 In locations where sufficient data is not available the proposed model cannot be used;



 The proposed model can be used for distinct multiple chemical sources (PCE, Benzene) at a locale by repeating the process for each chemical which shows a different finger print at the observation points.





Our Understanding of GW Modeling:

Groundwater flow modeling:

$$\frac{\partial \left(\phi s_{f} \rho_{f}\right)}{\partial t} = \nabla \cdot \left[\frac{\rho_{f} k_{m} k_{rf}}{\mu_{f}} \left(\nabla P_{f} + \rho_{f} g \nabla z\right)\right] + I_{f} \quad ; \quad f = w, g$$

Groundwater fate and transport modeling:

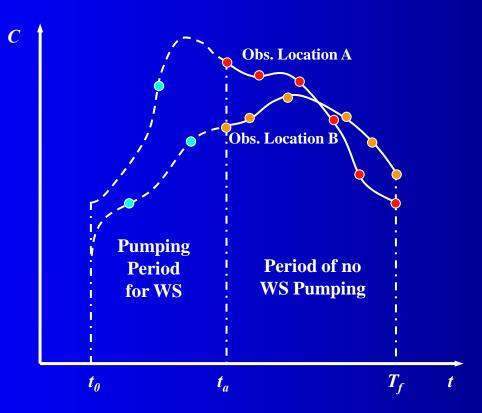
$$\frac{\partial \left(\phi s_{f} C_{f}^{i}\right)}{\partial t} = \nabla \left(\phi s_{f} D_{f}^{i} \nabla C_{f}^{i}\right) - \nabla \left(q_{f} C_{f}^{i}\right) \pm I_{f,MT}^{i} + I_{f,BT}^{i} + I_{source} \quad ; \quad f = w, g$$

• Matrix equations:

$$\left[\mathbf{M}\right]\frac{\partial\left\{C_{f}^{i}\right\}}{\partial t} = \left[\mathbf{S}\right]\left\{C_{f}^{i}\right\} \pm \sum\left\{F_{f}^{i}\right\} \quad ; \quad f = w, g$$



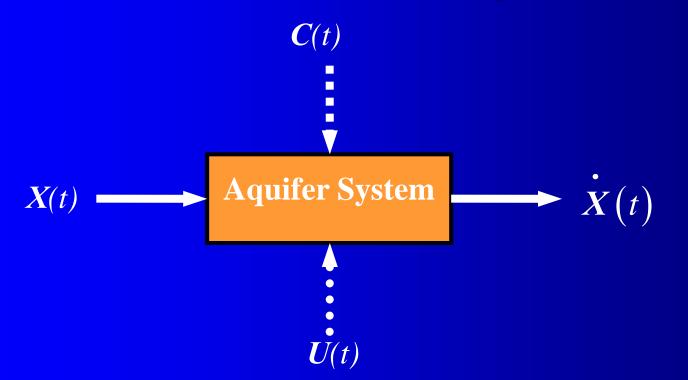
Available Data for Historical Reconstruction:







Idealization of the System:



 $X(t) = \begin{bmatrix} x_1(t), x_2(t), x_3(t), ..., x_i(t), ..., x_n(t) \end{bmatrix}^T$ $U(t) = \begin{bmatrix} u_1(t), u_2(t), u_3(t), ..., u_j(t), ..., u_m(t) \end{bmatrix}^T$ $C(t) = \begin{bmatrix} C_1(t), C_2(t), C_3(t), ..., C_i(t), ..., C_\ell(t) \end{bmatrix}^T$

Contaminant concentrations at monitoring wells

Pumping rates at wells

Contaminant concentrations at the source



$\begin{array}{l} \textbf{The Proposed Method:} \\ \textbf{X}(t) = \boldsymbol{\Phi} X(t) + \boldsymbol{\Psi} U(t) \\ \textbf{X}(t_0) = \textbf{X}_0 \end{array} \right\}$

matrix associated with aquifer parameters, BCs, contaminant \mathbf{O} is the $(n \times n)$ sources & fate etc. Ψ is the $(n \times m)$ matrix associated with pumping rates at extraction wells $\dot{X}(t)$ is the time derivative of the contaminant concentration vector at observation points X_0 is the initial contaminant concentration vector at the observation locations U(t)is the pumping rate vector at pumping locations



The Proposed Method:

If we use forward time integration:

 $\boldsymbol{X}(k+1) = \begin{bmatrix} \boldsymbol{\Phi} \Delta t + \mathbf{I} \end{bmatrix} \boldsymbol{X}(k) + \Delta t \, \boldsymbol{\Psi} \boldsymbol{U}(k) \\ \boldsymbol{X}(t_0) = \boldsymbol{X}_0$

$$\mathbf{A} = \begin{bmatrix} \mathbf{\Phi} \Delta t + \mathbf{I} \end{bmatrix}; \quad \mathbf{B} = \mathbf{\Psi} \Delta t$$

 $\boldsymbol{X}(k+1) = \boldsymbol{A}\boldsymbol{X}(k) + \boldsymbol{B}\boldsymbol{U}(k)$ $\boldsymbol{X}(t_0) = \boldsymbol{X}_0$



The Proposed Method:

• If we use backward time integration:

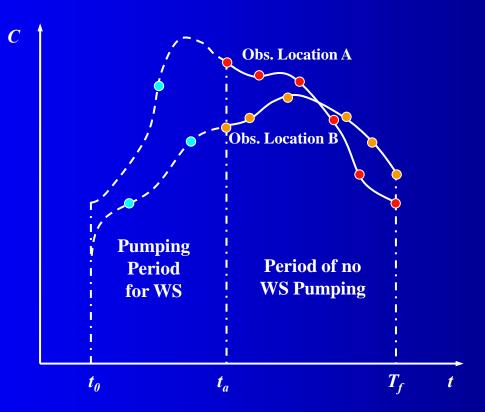
$$X(k) = \mathbf{A}^{-1}X(k+1) - \mathbf{A}^{-1}\mathbf{B}U(k)$$
$$X(T_f) = X_f$$
$$\mathbf{A}_b = \mathbf{A}\mathbf{B}^{1}; \quad \mathbf{B}_b = -\mathbf{A}^{-1}$$
$$X(k) = \mathbf{A}_b X(k+1) + \mathbf{B}_b U(k)$$

*** D R A F T - SUBJECT TO CHANGE ***

 $X(T_f) = X_f$



Data Available for Historical Reconstruction:







The Proposed Method: First Step X(k+1) = AX(k) + BU(k) $X(t_0) = X_0$

• For the period we have data from MW, we have U(k) = 0:

$$\boldsymbol{X}(k+1) = \boldsymbol{A} \boldsymbol{X}(k)$$

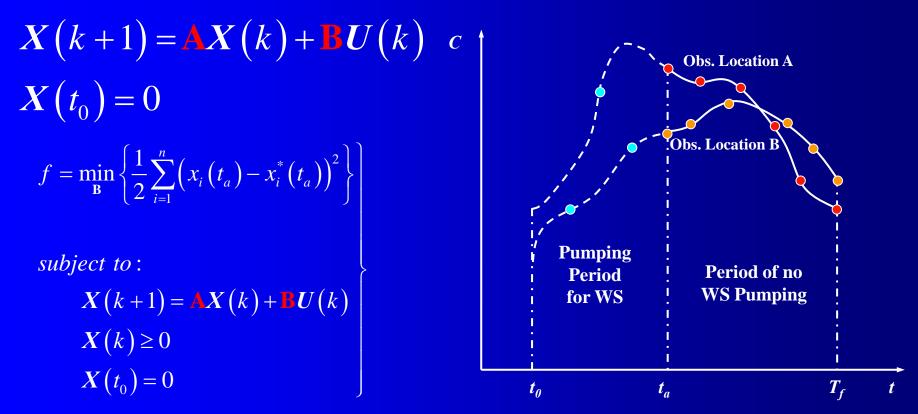
 Least squares method can be used to determine the coefficients of the matrix A





The Proposed Method: Second Step

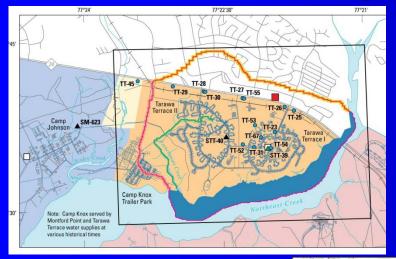
 Given the matrix A optimization methods can be used to determine the coefficients of the matrix B

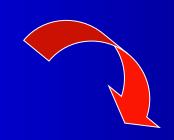


- The proposed method is based on these principles and algorithms



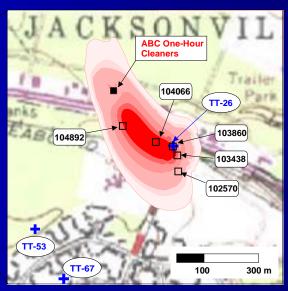
Verification Study: Tarawa Terrace Data

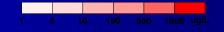






Three pumping wells: TT-26, TT-53, and TT-67
Five monitoring points.

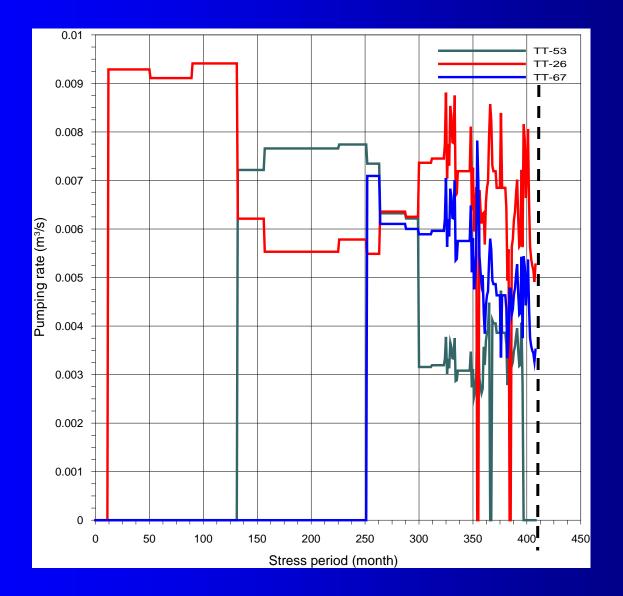




PCE concentration distribution in December 1984 (stress period=408) at z = -24 m.

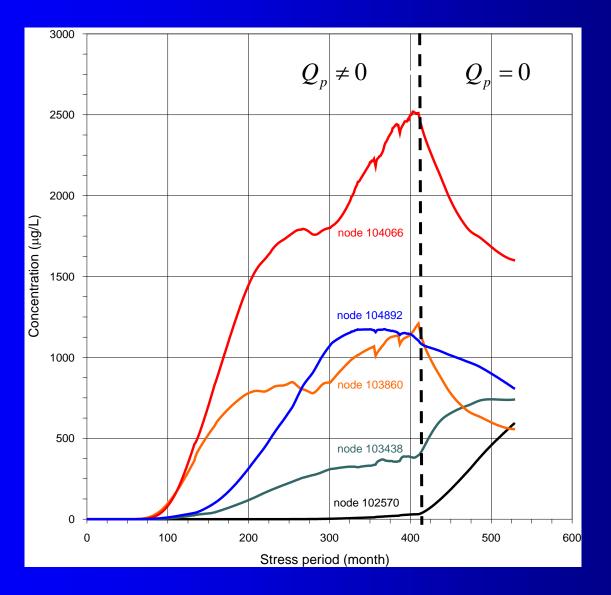


Tarawa Terrace Pumping Schedule:



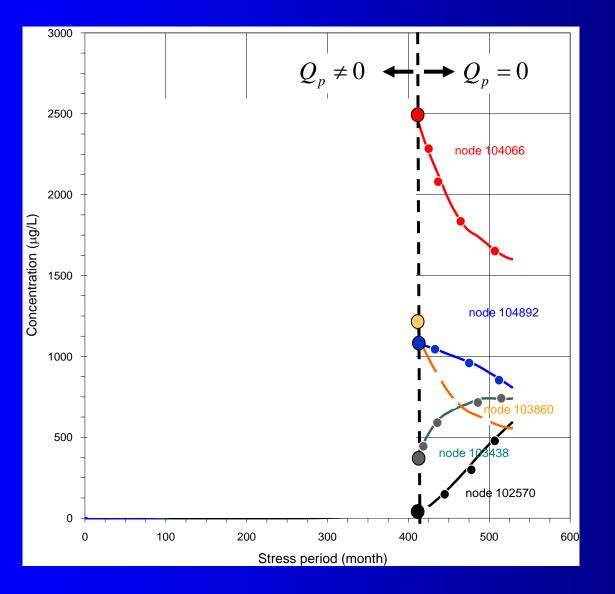


Tarawa Terrace Data:



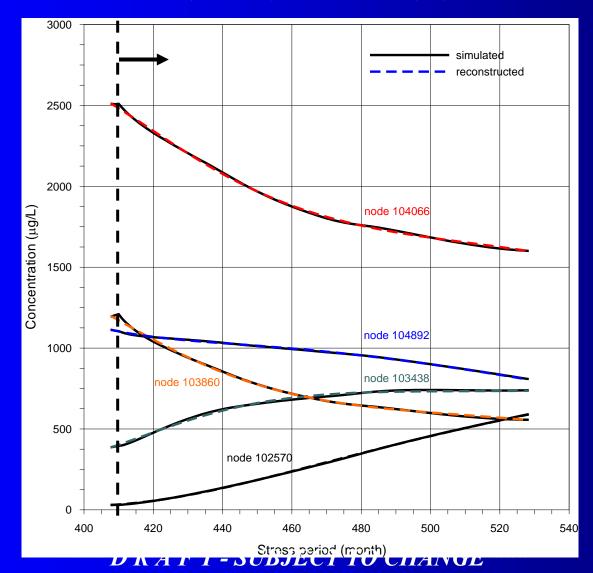


Tarawa Terrace Data:



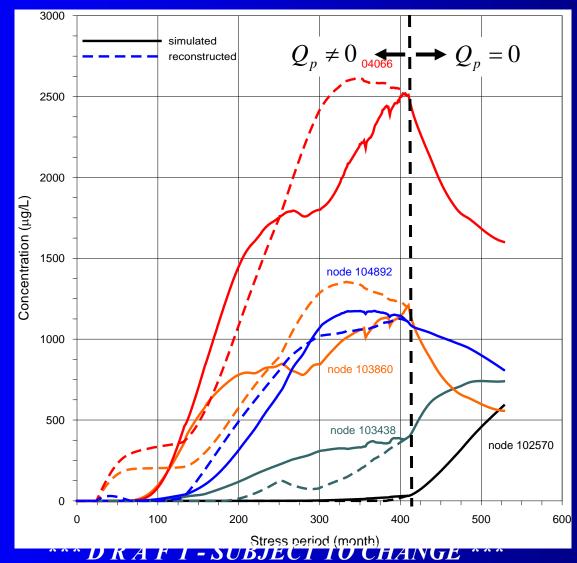


Tarawa Terrace Outcome: LSM X(k+1) = A X(k)



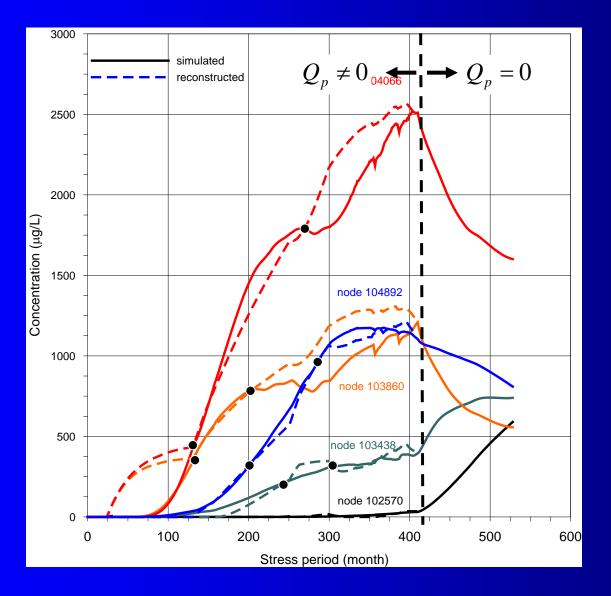


Tarawa Terrace Outcome (FW – 0 Int. points): $X(k+1) = \mathbf{A}X(k) + \mathbf{B}U(k)$



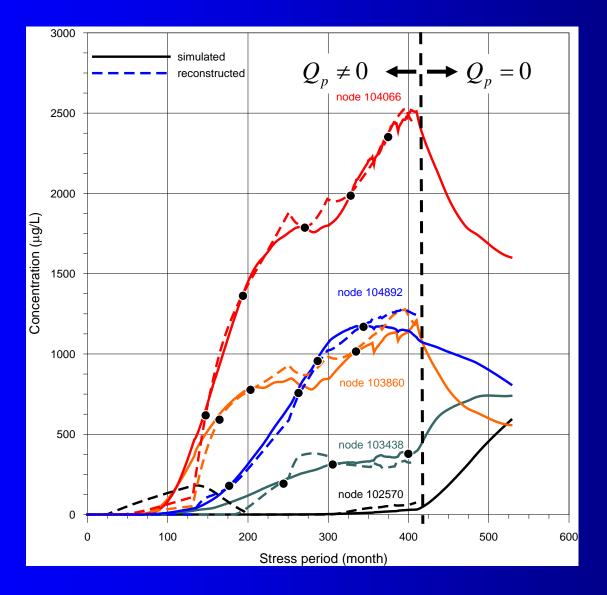


Tarawa Terrace Outcome (FW – 8 Int. Points):



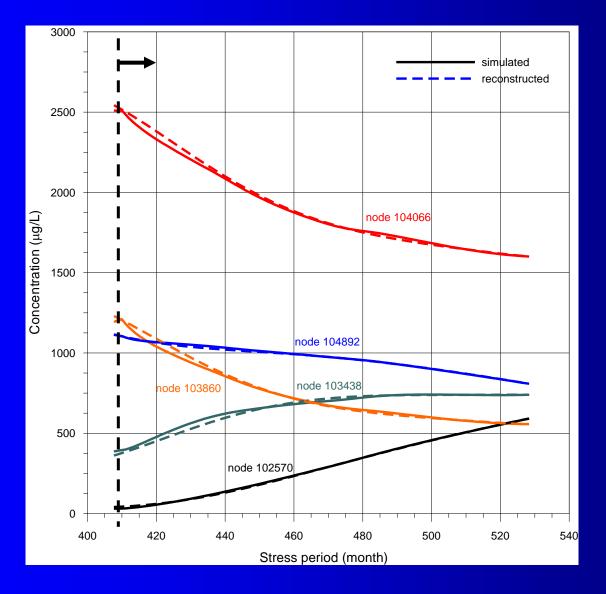


Tarawa Terrace Outcome (FW – 15 Int. Points):



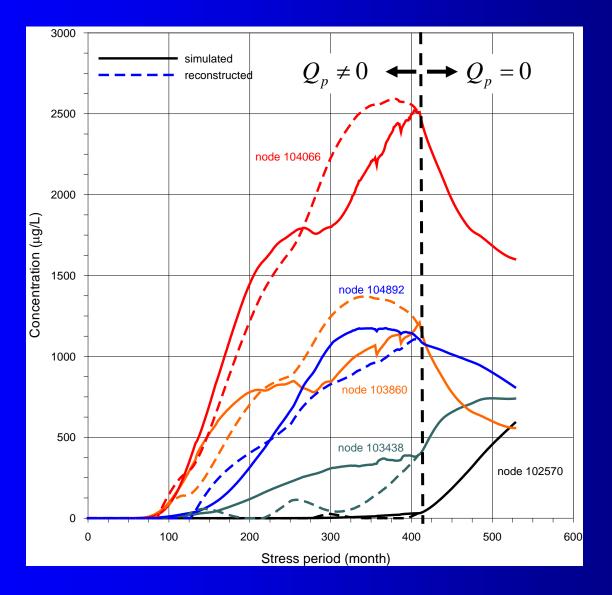


Tarawa Terrace Outcome (BW):



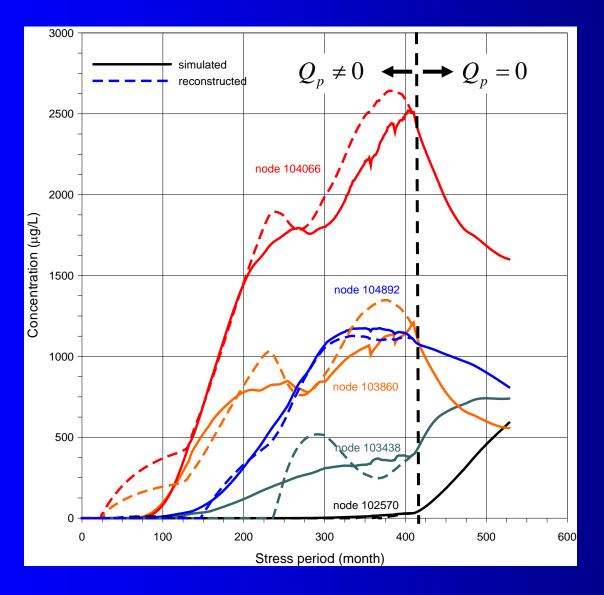


Tarawa Terrace Outcome (BW – 0 Int. Points):



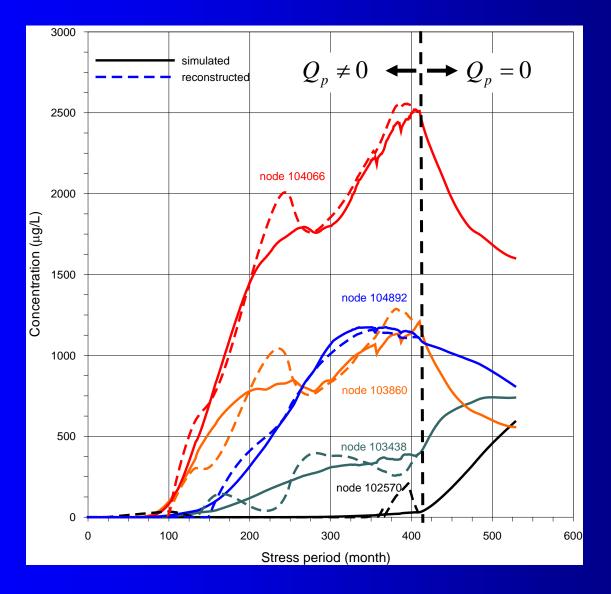


Tarawa Terrace Outcome (BW – 8 Int. Points):





Tarawa Terrace Outcome (BW – 15 Int. Points):



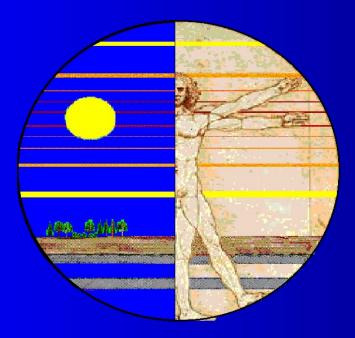


Extended procedures:

- The use of FW and BW procedures iteratively to improve on solution;
- Introduction of Kalman filtering method to evaluate the effect of data and computational algorithm error on the solution and establish confidence bands on the solutions obtained; and,
- Application of the method to Hadnot Point aquifers.







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