PCE Exposure Reconstruction for Camp Lejeune, NC Epidemiologic Study:  
The Effect of Historical Supply-Well Schedule Variation on PCE Arrival Time  

* Multimedia Environmental Simulations Laboratory, Georgia Institute of Technology  
** Agency for Toxic Substances and Disease Registry  
*** R.E. Faye and Associates  

ASCE, World Environmental & Water Resources Conference  
Tampa, Florida  
05/15/07
Background

Epidemiologic study at Camp Lejeune, NC

(lack of exposure data)

Historical reconstruction of contaminant fate and transport
Background
The graph visualizes the concentration of PCE (Perchloroethylene) over time from January 1951 to January 1987. The concentrations are shown on a logarithmic scale, indicating that the data spans several orders of magnitude. Each line represents a different sample or well, labeled as TT-26, TT-25, TT-53, TT-23, TT-67, TT-31A, TT-31B, TT-54A, TT-54B, and WTP (Water Treatment Plant). The PCE MCL (Maximum Contaminant Level) for PCE is also indicated, with a horizontal line at a concentration of 1000 ppb (parts per billion). The summation formula for the overall concentration at time $t$, $C_t$, is shown:

$$C_t = \frac{\sum_{i=1}^{N} Q_{it}C_{it}}{\sum_{i=1}^{N} Q_{it}}$$

Where $Q_{it}$ represents the flow rate of the $i$th component at time $t$, and $C_{it}$ is the concentration of the $i$th component at time $t$. The dates of interest are marked as 01/1957 and 11/1957, indicating significant changes or events at these times.
Background

Epidemiologic study at Camp Lejeune, NC
(lack of exposure data)

Historical reconstruction of contaminant fate and transport
(uncertainties)

Sensitivity and uncertainty analysis
(study of pumping schedule only)

The effect of historical supply-well schedule variation on PCE arrival time at pumping wells and water treatment plant
Goal & Approach

➢ **Goal**
  ➢ Evaluation of the earliest and the latest arrival times of contaminant at the water treatment plant (WTP) as a function of pumping schedules.

➢ **Assumptions**
  ➢ Pumping demand at each Stress Period is constant.
  ➢ Pumping schedules are the only variables.
  ➢ PCE is the only contaminant studied.

➢ **Approach**
  ➢ Coupling of simulation models (MODFLOW, MT3DMS) and special optimization techniques as developed in this study.
Analysis of Problem

Conversion of problem:

- Easier to calculate by using MT3DMS.
- Arrival time of any concentration level can be determined as an output.

Simplifications:

- Optimize pumping schedules for max./min. concentration arrival time at each Stress Period.
- Theoretically applicable but practically infeasible due to computational limitations.
  - The large simulation system (528 Stress Periods, 200X270X7 Nodes) requires long simulation time.
Optimization Model

Max $C_i = f(u_i)$
$s.t.$
$0 \leq u_i \leq w_i$

$\sum_{j=1}^{n} u_{ij} = Q_{Ti}$

$u_k = u^*_k \ (k = 1,...,i-1)$

where
$C_i$: average contaminant concentration in the water treatment plant;
$u_i$: n dimensional vector of pumping rates at stress period $i$;
$w_i$: n dimensional vector of upper bound of $u_i$ at stress period $i$;
$Q_{Ti}$: total water demand at stress period $i$;
$u^*_k$: optimal pumping schedule for stress period $k$. 
Optimization Techniques

- Traditional non-linear optimization methods:
  - The solution may tend to be a local optimum.
  - Computationally demanding.
    - Gradient information may be required.
    - Number of iterations may be needed for optimal solution.

- Genetic Algorithm (GA):
  - “Claimed” to have global optimizing ability.
  - Computationally demanding.
    - A 4-well, 3-stress period problem requires a GA simulation with a population size of 200 to run 270 generations to converge.

- Proposed approach:
  - Improved gradient method based on Rank-and-Assign.
PSOpS Algorithm

1. Calculate $C_i^{(0)}$ and $(\partial C_i / \partial q_i)^{(0)}$, sort $(\partial C_i / \partial q_i)^{(0)}$ for $SQ_i^{(0)}$

2. $\nabla C_i(q_i^{(0)}) \leq \varepsilon^3$
   - Yes: Stop
   - No: Create $q_i^{(1)}$ according to $SQ_i^{(0)}$, $w_i$ and $Q_i$

3. Calculate $C_i^{(1)}$ and $(\partial C_i / \partial q_i)^{(1)}$, sort $(\partial C_i / \partial q_i)^{(1)}$ for $SQ_i^{(1)}$

4. $SQ_i^{(0)} = SQ_i^{(1)}$?
   - Yes: Stop
   - No: $\nabla C_i(q_i^{(1)}) \leq \varepsilon^3$

5. Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, $w_i$ and $Q_i$

6. $q_i^{(1)} = q_i^{(2)}$?
   - Yes: Stop
   - No: $C_i^{(1)} = C_i^{(2)}$

7. $SQ_i^{(0)} = SQ_i^{(2)}$?
   - Yes: Stop
   - No: $C_i^{(0)} < C_i^{(2)}$

8. Improved Gradient method

9. Save result, go to next S.P.
PSOpS Algorithm

- Calculate $C_i^{(0)}$ and $\frac{\partial C_i^{(0)}}{\partial q_i}$, sort $\frac{\partial C_i^{(0)}}{\partial q_i}$ for $SQ_i^{(0)}$
- $\|V C_i(q_i^{(0)})\| < \epsilon$?
  - Yes
  - No
- Create $q_i^{(1)}$ according to $SQ_i^{(0)}$, $w_i$ and $Q_i$
- Calculate $C_i^{(1)}$ and $\frac{\partial C_i^{(1)}}{\partial q_i}$, sort $\frac{\partial C_i^{(1)}}{\partial q_i}$ for $SQ_i^{(1)}$
- $SQ_i^{(0)} = SQ_i^{(1)}$?
  - Yes
  - No
- $\|V C_i(q_i^{(1)})\| < \epsilon$?
  - Yes
  - No
- Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, $w_i$ and $Q_i$
- $q_i^{(1)} = q_i^{(2)}$?
  - Yes
  - No
- $C_i^{(0)} = C_i^{(1)}$, $q_i^{(1)} = q_i^{(2)}$, $SQ_i^{(0)} = SQ_i^{(1)}$

- Improved Gradient method
- Save result, go to next S.P.

If every variable is same as previous SP, the optimized pumping schedule (PS) and well sequence (SQ) from previous solution will be selected.
PSOpS Algorithm

Calculate $C^{(0)}_i$ and $\frac{\partial C}{\partial q_i}^{(0)}$, sort $\frac{\partial C}{\partial q_i}^{(0)}$ for $SC^{(0)}$

$\|\nabla C(q_i^{(0)})\| < \epsilon^T$

Create $q_i^{(1)}$ according to $SC^{(0)}$, $w_i$ and $Q_n$

Calculate $C^{(1)}_i$ and $\frac{\partial C}{\partial q_i}^{(1)}$, sort $\frac{\partial C}{\partial q_i}^{(1)}$ for $SC^{(1)}$

$SC^{(0)} = SC^{(1)}?$

$\|\nabla C(q_i^{(1)})\| < \epsilon^T$

Create $q_i^{(2)}$ according to $SC^{(1)}$, $w_i$ and $Q_n$

$q_i^{(0)} = q_i^{(1)}?$

$C^{(0)}_i = C^{(1)}_i$, $q_i^{(1)} = q_i^{(2)}$  
$SC^{(0)} = SC^{(1)}$

$C^{(0)} < C^{(1)}?$

Improved Gradient method

Save result, go to next S.P.
PSOpS Algorithm

Calculate $C_i^{(0)}$ and $\frac{\partial C_i}{\partial q_i}$, sort $\frac{\partial C_i}{\partial q_i}$ for $SQ_i^{(0)}$

$\|\nabla C_i(q_i^{(0)})\| < \varepsilon^3$

Create $q_i^{(0)}$ according to $SQ_i^{(0)}$, $w_i$ and $Q_i$.

Calculate $C_i^{(1)}$ and $\frac{\partial C_i}{\partial q_i}$, sort $\frac{\partial C_i}{\partial q_i}$ for $SQ_i^{(1)}$

$SQ_i^{(1)} = SQ_i^{(0)}$?

$\|\nabla C_i(q_i^{(1)})\| < \varepsilon^3$

Create $q_i^{(1)}$ according to $SQ_i^{(0)}$, $w_i$ and $Q_i$.

$C_i^{(0)} = C_i^{(1)}$, $q_i^{(1)} = q_i^{(2)}$

$SQ_i^{(0)} = SQ_i^{(1)}$

Improved Gradient method

Save result, go to next S.P.

If $SQ_1 = SQ_2$, optimization process takes only two iterations, which is more efficient than traditional methods.

This process is intuitive (+ wells are at full capacity, - wells are at partial capacity).

Mathematical convergence is also proven.
PSOpS Algorithm

Calculate $C^{(0)}$ and $\frac{\partial C^{(0)}}{\partial q_i}$, sort $\frac{\partial C^{(0)}}{\partial q_i}$ for $SQ^{(0)}$

\[ \| \nabla C_i(q_i^{(0)}) \| \leq \varepsilon ? \]

Create $q_i^{(0)}$ according to $SQ^{(0)}$, $w_i$ and $Q_i$

Calculate $C^{(1)}$ and $\frac{\partial C^{(1)}}{\partial q_i}$, sort $\frac{\partial C^{(1)}}{\partial q_i}$ for $SQ^{(1)}$

$SQ^{(0)} = SQ^{(1)}$?

\[ \| \nabla C_i(q_i^{(1)}) \| \leq \varepsilon ? \]

Create $q_i^{(1)}$ according to $SQ^{(1)}$, $w_i$ and $Q_i$

$C^{(0)} = C^{(1)}$, $q_i^{(0)} = q_i^{(1)}$?

$SQ^{(0)} = SQ^{(1)}$?

Improved Gradient method

Save result, go to next S.P.
PSOpS Algorithm

Even if Improved Gradient method is required, the optimization process works on wells that have different rankings only, thus computationally less demanding.
PSOpS Algorithm

At the end of each SP, head and conc. are saved and chosen to be the starting points for simulation of the next SP. Thus we avoid repeating the simulation from SP1 again and this saves computation cost.
Example of a PSOpS Process

1. Calculate $C_i^{(0)}$ and $\frac{\partial C_i^{(0)}}{\partial q_i}$, sort $\frac{\partial C_i^{(0)}}{\partial q_i}$ for $SQ^{(0)}$.

2. If $\|\nabla C_i(q_i^{(0)})\| < \varepsilon$ then:
   - If $SQ^{(0)} = SQ^{(0)}$ then:
     - If $\|\nabla C_i(q_i^{(0)})\| < \varepsilon$ then:
       - Create $q_i^{(2)}$ according to $SQ^{(0)}$, $w_i$ and $Q_i$.
     - If $q_i^{(1)} = q_i^{(1)}$ then:
       - $C_i^{(0)} = C_i^{(1)}$, $q_i^{(1)} = q_i^{(2)}$, $SQ^{(0)} = SQ^{(1)}$.
     - If $C_i^{(0)} < C_i^{(1)}$ then:
       - Improved Gradient method
   - If $q_i^{(1)} = q_i^{(1)}$ then:
     - $q_i^{(1)} = q_i^{(1)}$.

3. If $\# of cases$ then:
   - Total: $422$
PCE Distribution under Different Schedules
PCE Conc. under Different Schedules

Original Schedule

Minimum Schedule I

Maximum Schedule

Minimum Schedule II

TT-26
TT-25
TT-53
TT-23
TT-67
TT-31A
TT-31B
TT-54A
TT-54B
TT-67A
TT-67B
PCE MCL
PCE Conc. in WTP and PR in TT-26
Evaluation Results

<table>
<thead>
<tr>
<th>Schedule</th>
<th>Org.</th>
<th>Max.</th>
<th>Min. I</th>
<th>Min. II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Conc. (ppb)</td>
<td>183.04</td>
<td>304.66</td>
<td>41.36</td>
<td>45.31</td>
</tr>
<tr>
<td>Total Mass Out (g)</td>
<td>2.45E6</td>
<td>4.59E6</td>
<td>1.98E5</td>
<td>3.41E5</td>
</tr>
<tr>
<td>Total Mass Released (g)</td>
<td>1.40E7</td>
<td>1.40E7</td>
<td>1.40E7</td>
<td>1.40E7</td>
</tr>
<tr>
<td>Out/Released (%)</td>
<td>17.50</td>
<td>32.78</td>
<td>1.41</td>
<td>2.44</td>
</tr>
</tbody>
</table>
Conclusions

- The PCE MCL arrival time in WTP at Tarawa Terrace could be between 12/1956 to 06/1960.

- The PCE concentration in WTP at Tarawa Terrace could vary by several magnitudes depending on pumping schedule.

- Because of its location (vicinity and downstream to contaminant source), well TT-26 has played a crucial role in fate and transport of PCE.

- All results are based on specified pumping demands and pumping capacities. Uncertainty in those parameters are not considered.
Summary

- A pumping schedule optimization method for large groundwater system with numerous simulation stress periods has been developed using an improved gradient method.

- The system has been successfully applied to Camp Lejeune study to determine the pumping schedules for max./min. PCE concentration arrival times to the WTP.

- The method has proven to be computationally efficient.
Thank you