The Effect of Historical Supply-Well Schedule Variation on PCE Arrival Time

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** Agency for Toxic Substances and Disease Registry
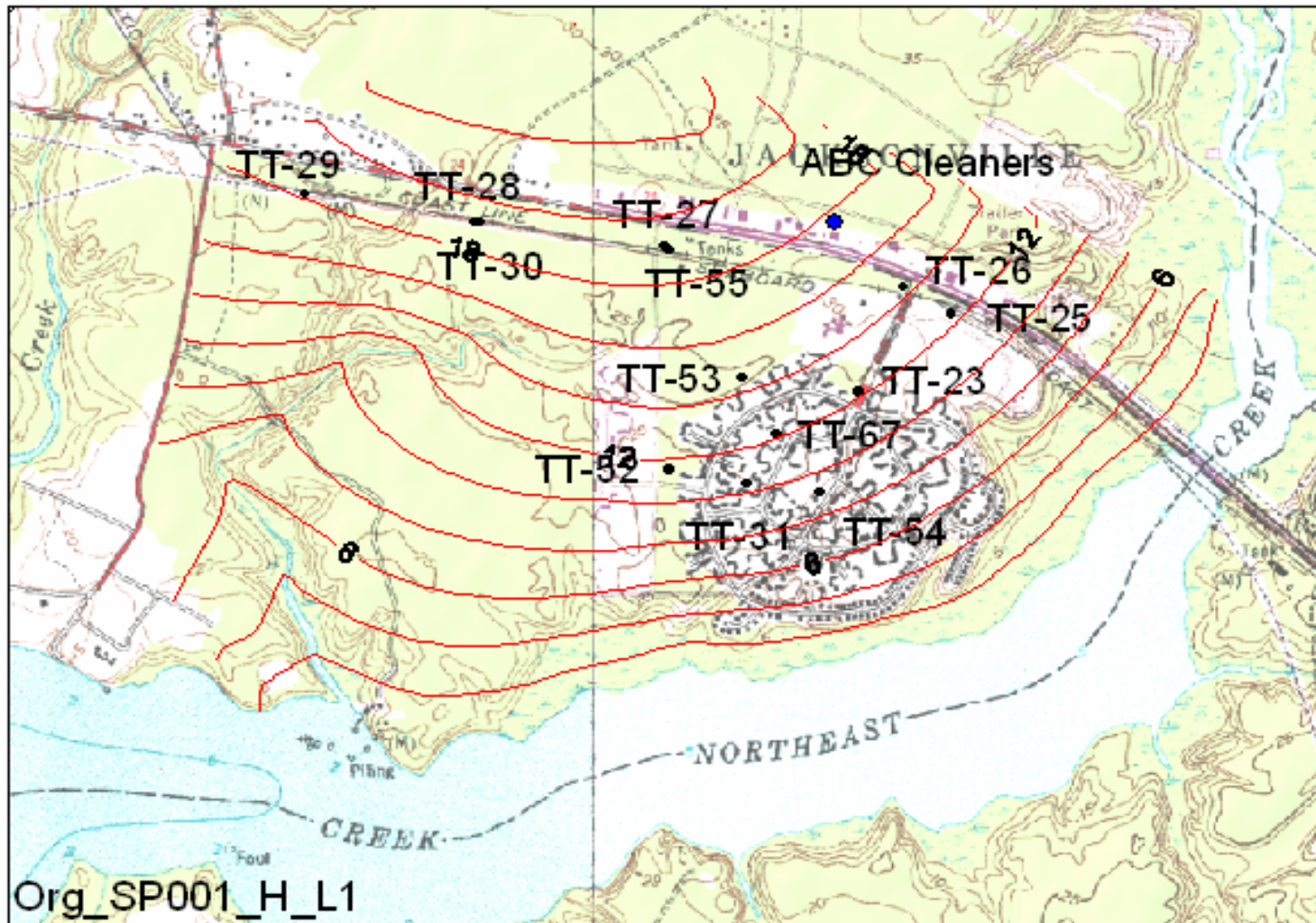
*** R.E. Faye and Associates

Background

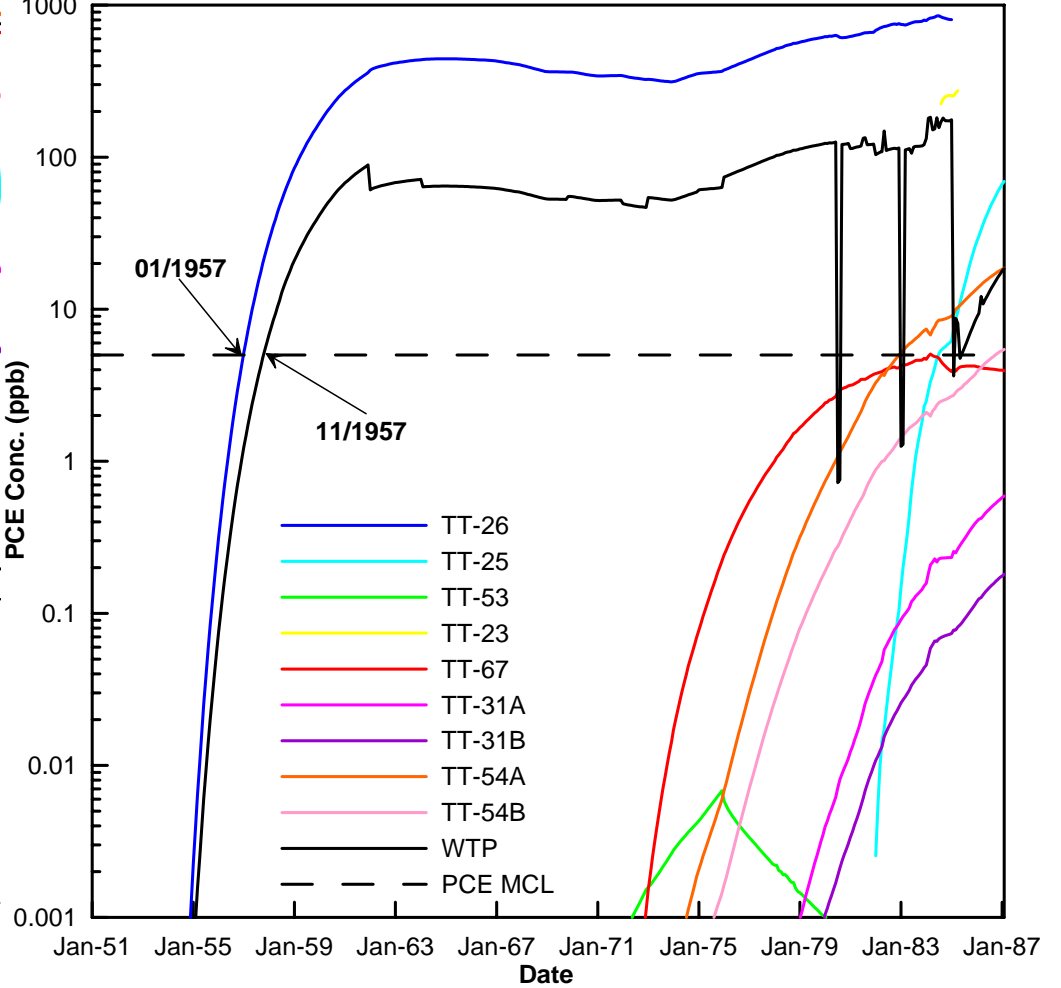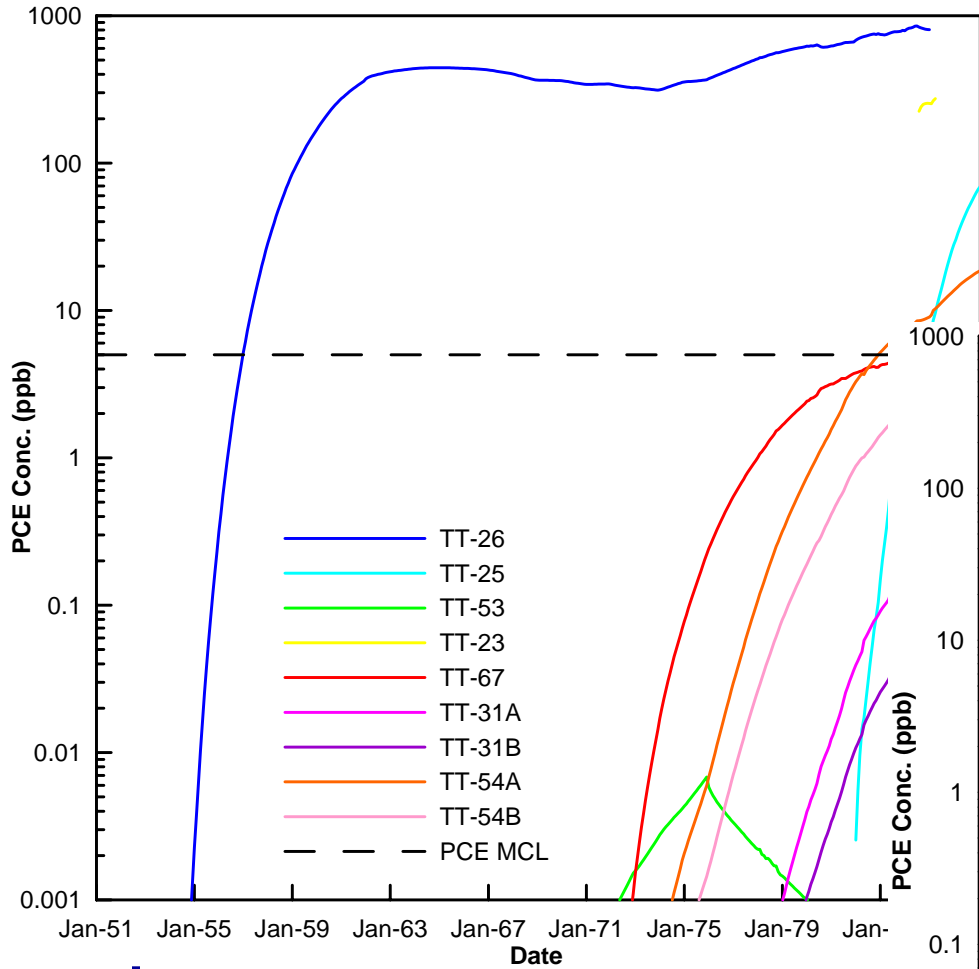Epidemiologic study at Camp Lejeune, NC

(lack of exposure data)

Historical reconstruction of contaminant fate and transport

Background

$$C_t = \frac{\sum\limits_{i=1}^{N} Q_{it} c_{it}}{\sum\limits_{i=1}^{N} Q_{it}}$$

Background

Epidemiologic study at Camp Lejeune, NC

(lack of exposure data)

Historical reconstruction of contaminant fate and transport

(uncertainties)

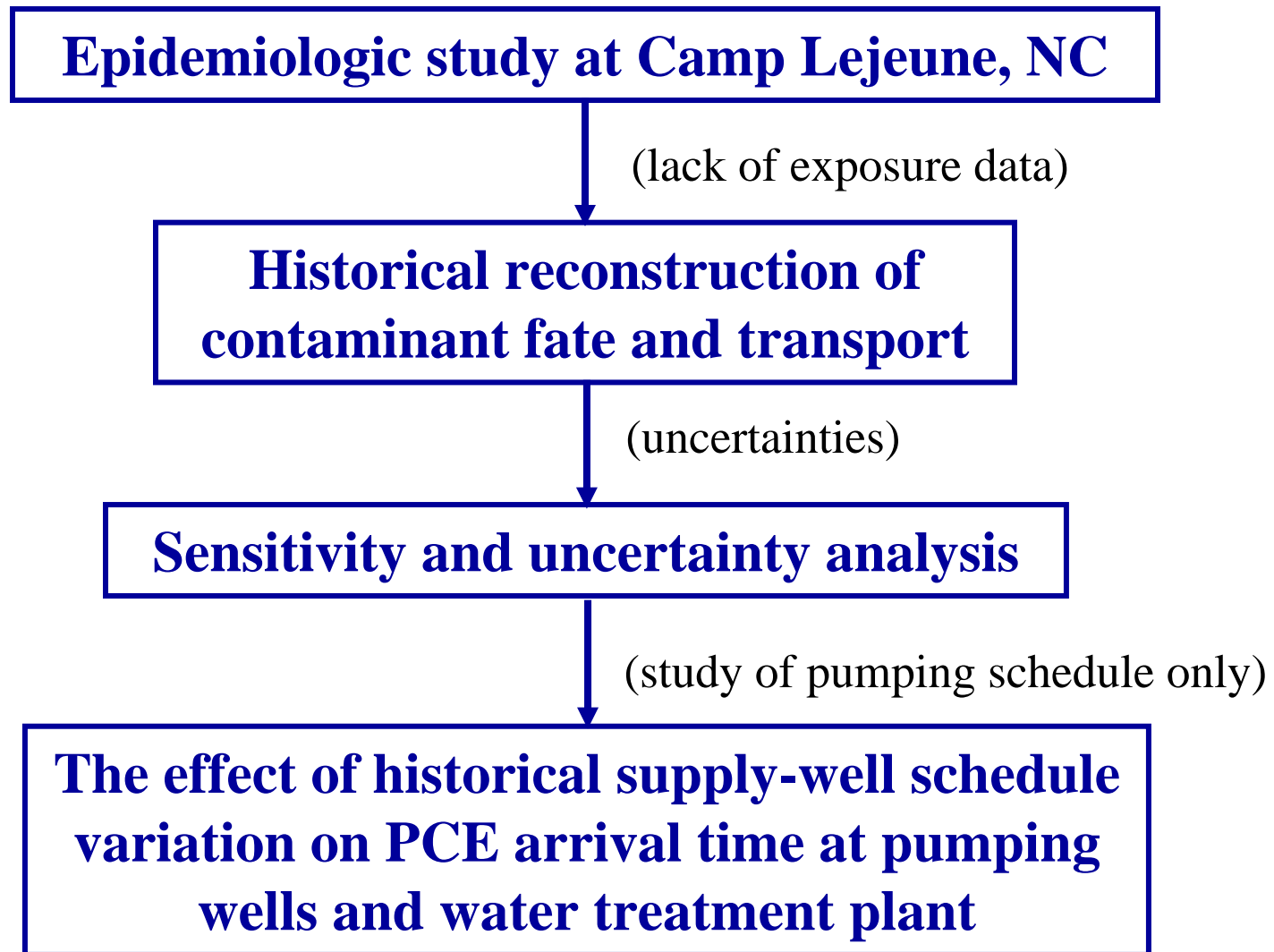Sensitivity and uncertainty analysis

(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.
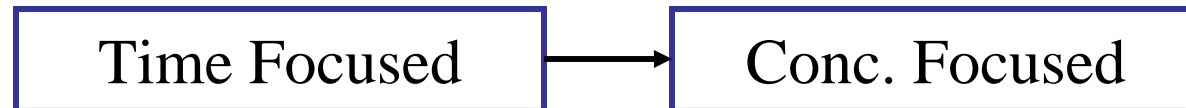
  ➢ PCE is the only contaminant studied.

➢ **Approach**

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

Analysis of Problem

➢ **Conversion of problem:**

Time Focused	→	Conc. Focused

   ➢ 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

$$\underset{u_i \in R^n}{Max} \ C_i = f(u_i)$$

$$s.t.$$

$$0 \le u_i \le w_i$$

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

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

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;

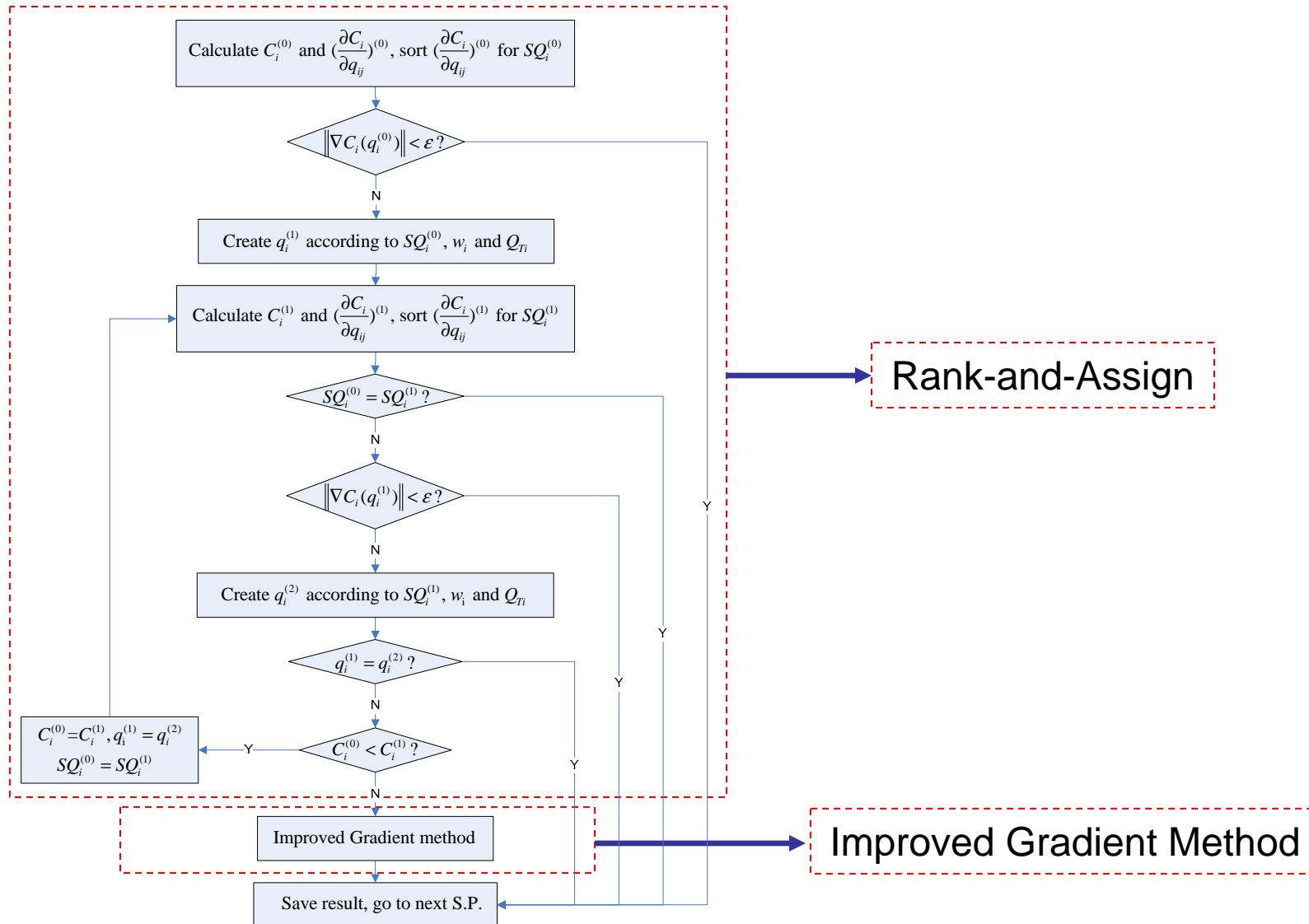u_k^* : optimal pumping schedule for stress period k.
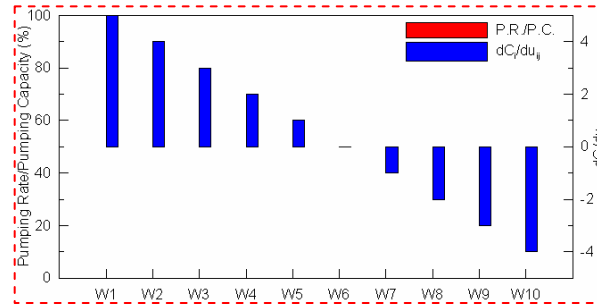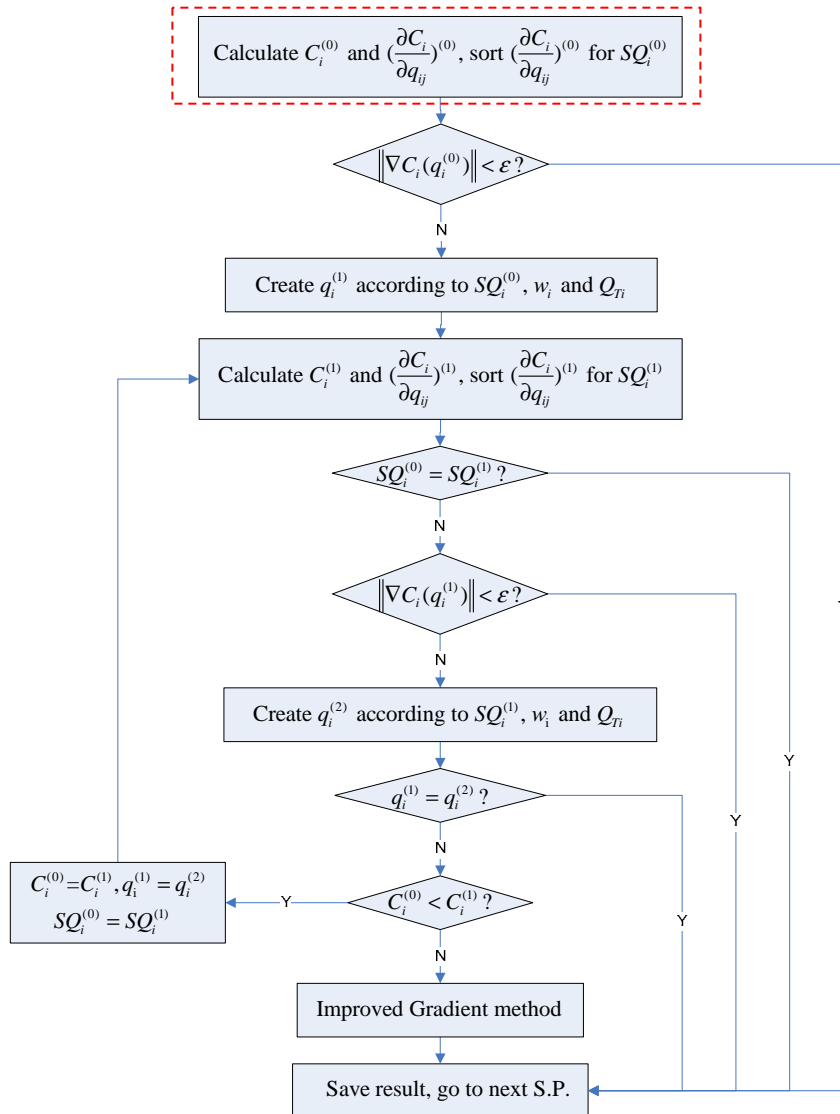
Optimization Techniques

➢ **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

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

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

N

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

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

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

N

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

N

Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, w_i and Q_{Ti}

$q_i^{(1)} = q_i^{(2)}$?

N

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

Y

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

N

Y

Y

Y

Y

Improved Gradient method

Save result, go to next S.P.

Rank-and-Assign

Improved Gradient Method

PSOpS Algorithm

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

$\left\| \nabla C_i(q_i^{(0)}) \right\| < \varepsilon$?

N

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

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

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

N

$\left\| \nabla C_i(q_i^{(1)}) \right\| < \varepsilon$?

N

Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, w_i and Q_{Ti}

$q_i^{(1)} = q_i^{(2)}$?

N

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

$C_i^{(0)} < C_i^{(1)}$? Y

N

Improved Gradient method

Save result, go to next S.P.

Y

If every variable is same as previous SP, the optimized pumping schedule (PS) and well sequence (SQ) from previous solution will be selected.
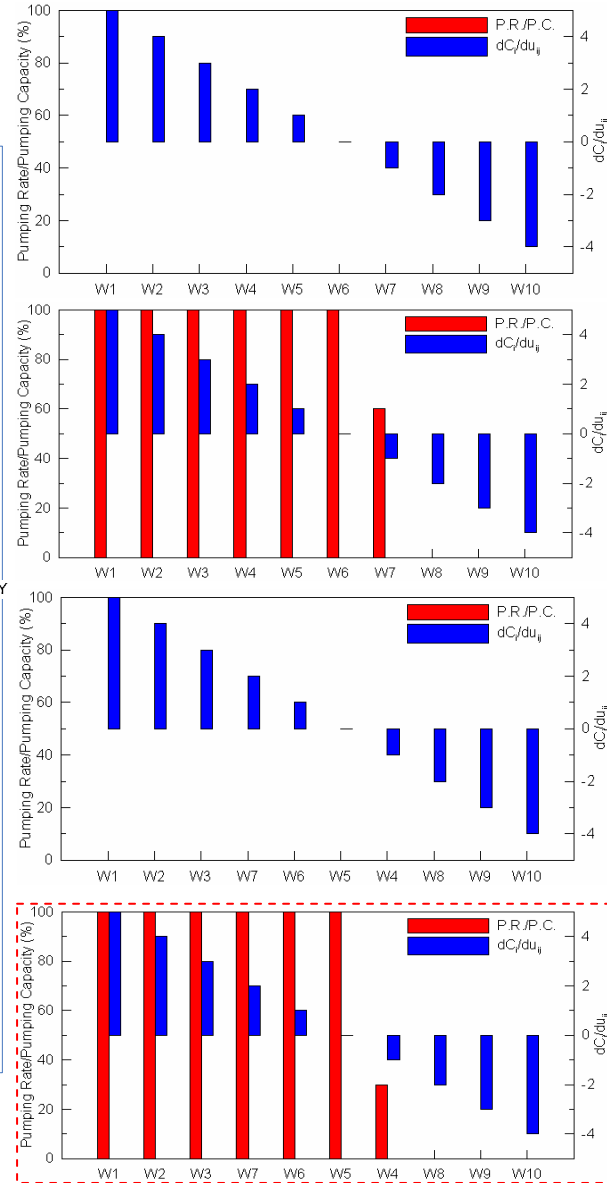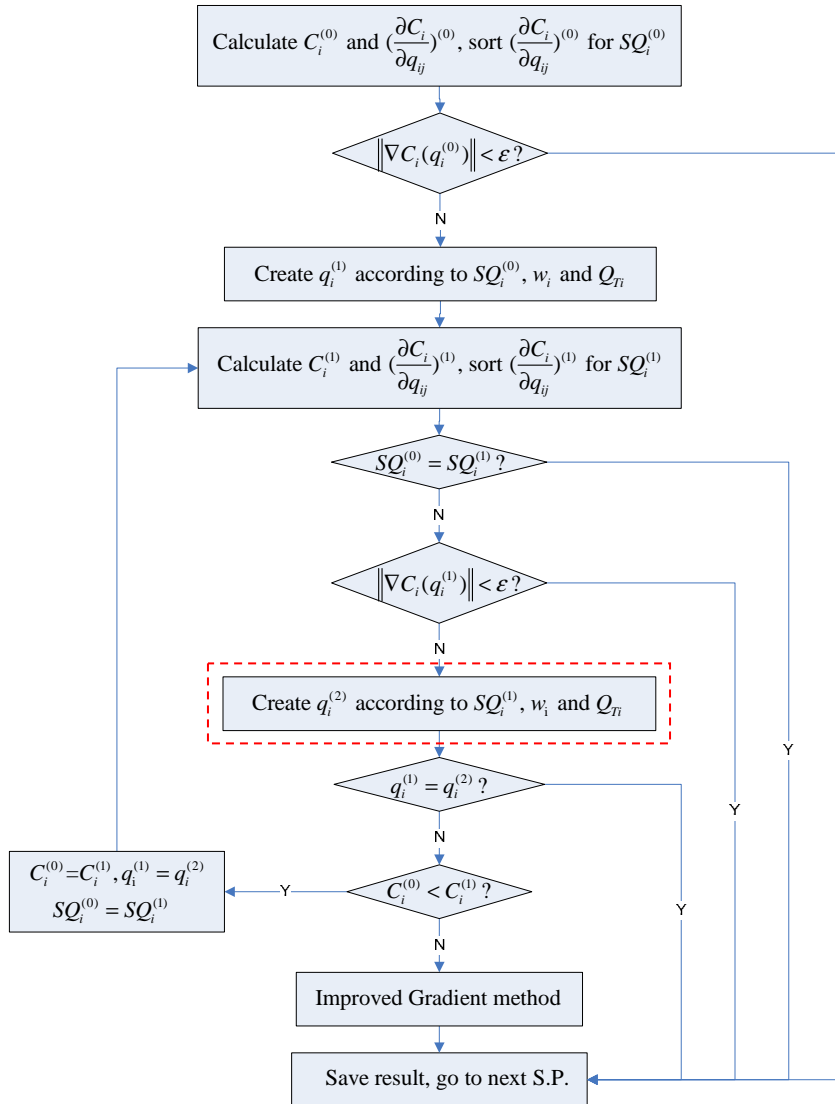
PSOpS Algorithm
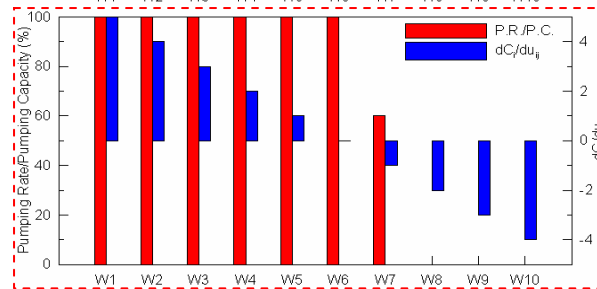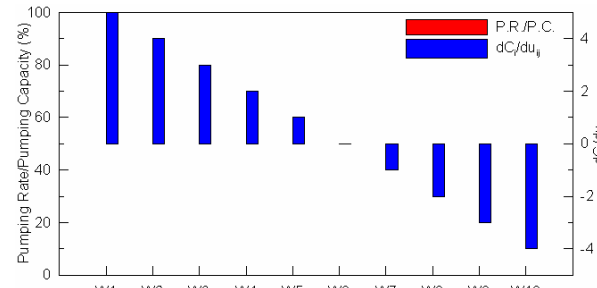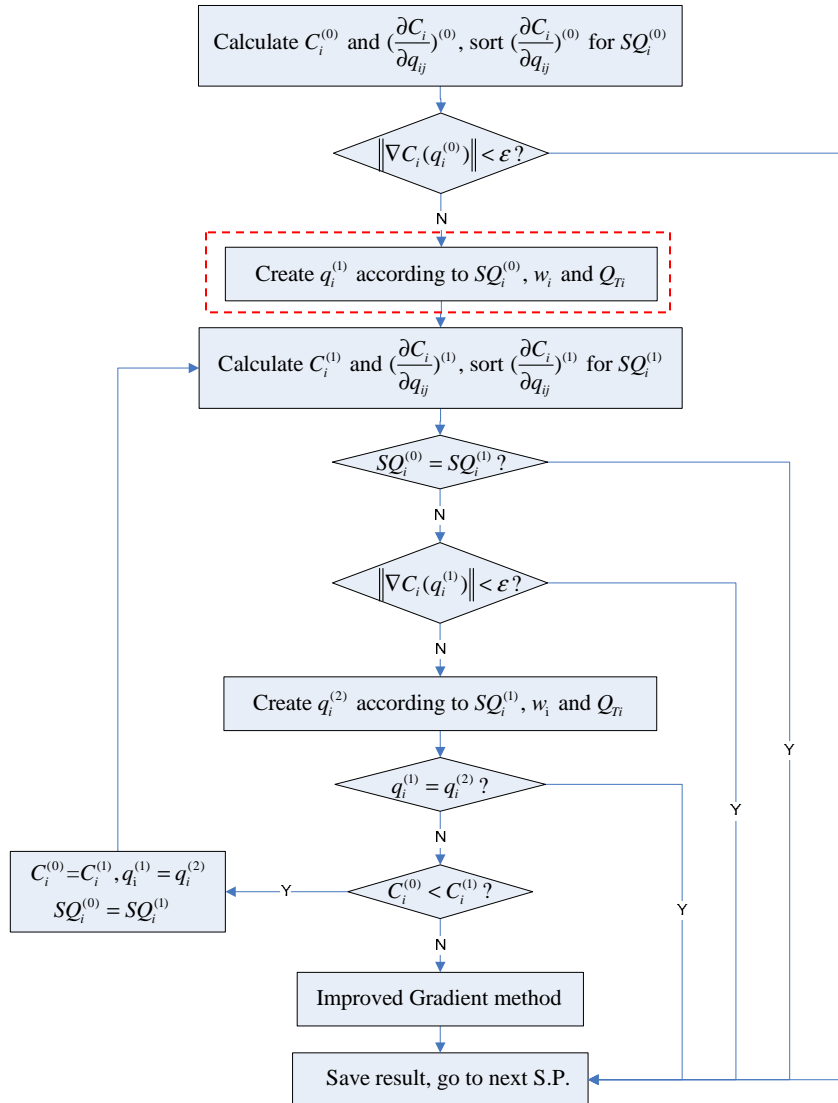
PSOpS Algorithm
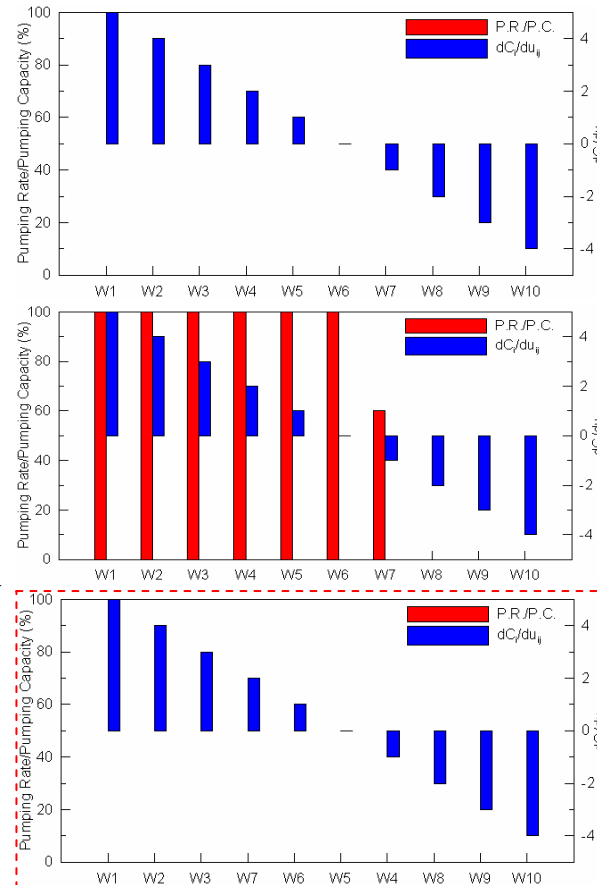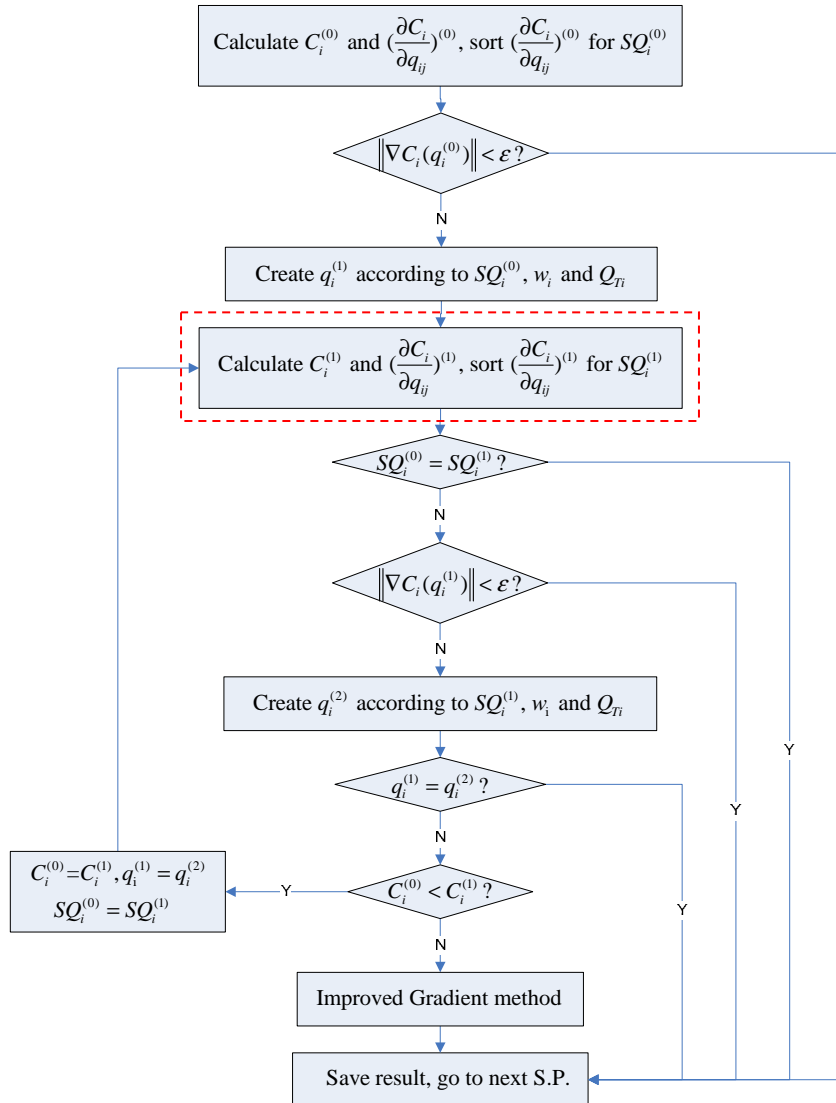
If $SQ_1 = SQ_2$, optimization process takes only two iterations, which is more efficient than traditional methods.

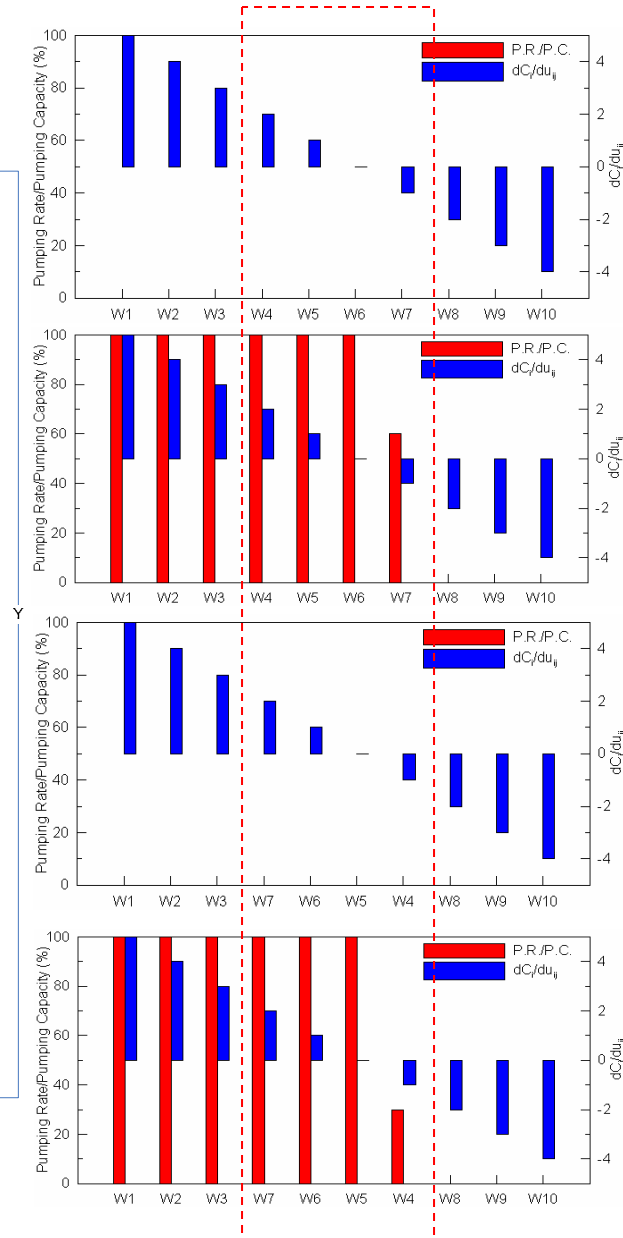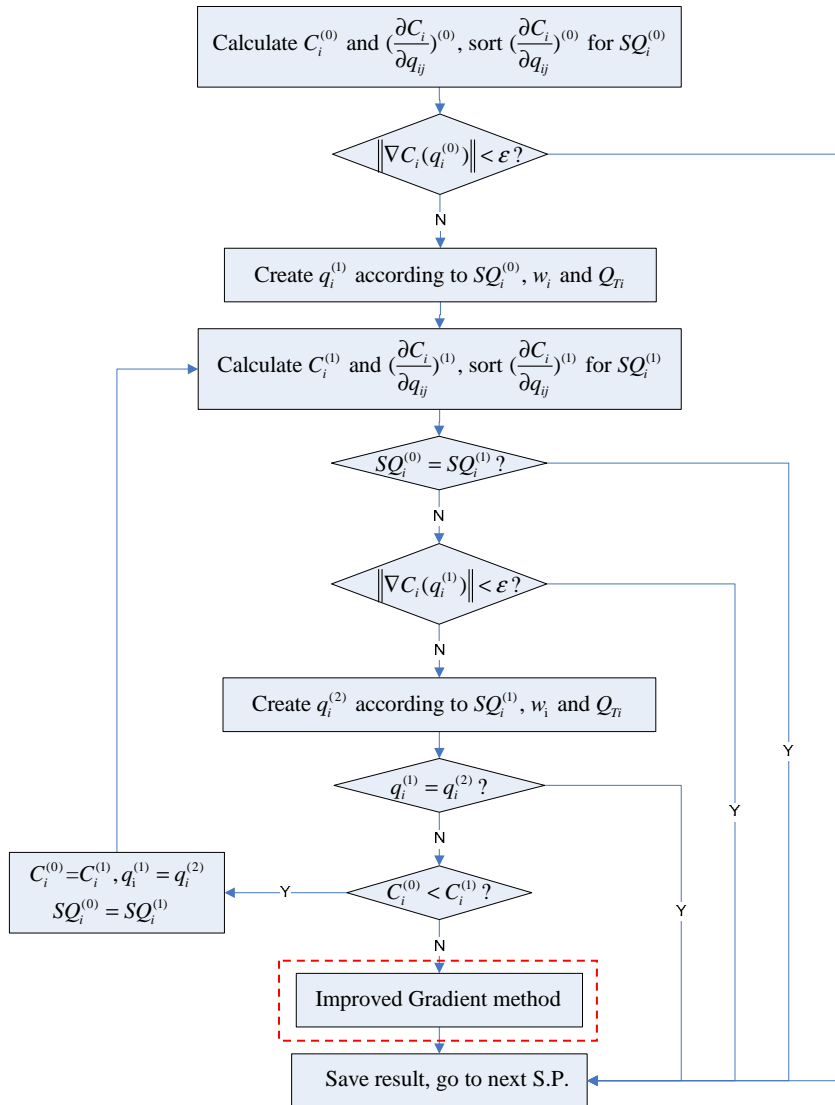This process is intuitive (+ wells are at full capacity, - wells are at partial capacity).

Mathematical convergence is also proven.

PSOpS Algorithm

PSOpS Algorithm

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

$\left\| \nabla C_i(q_i^{(0)}) \right\| < \varepsilon$?

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

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

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

$\left\| \nabla C_i(q_i^{(1)}) \right\| < \varepsilon$?

Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, w_i and Q_{Ti}

$q_i^{(1)} = q_i^{(2)}$?

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

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

Improved Gradient method

Save result, go to next S.P.

Even if Improved Gradient method is required, the optimization process works on wells that have different rankings only, thus computationally less demanding.
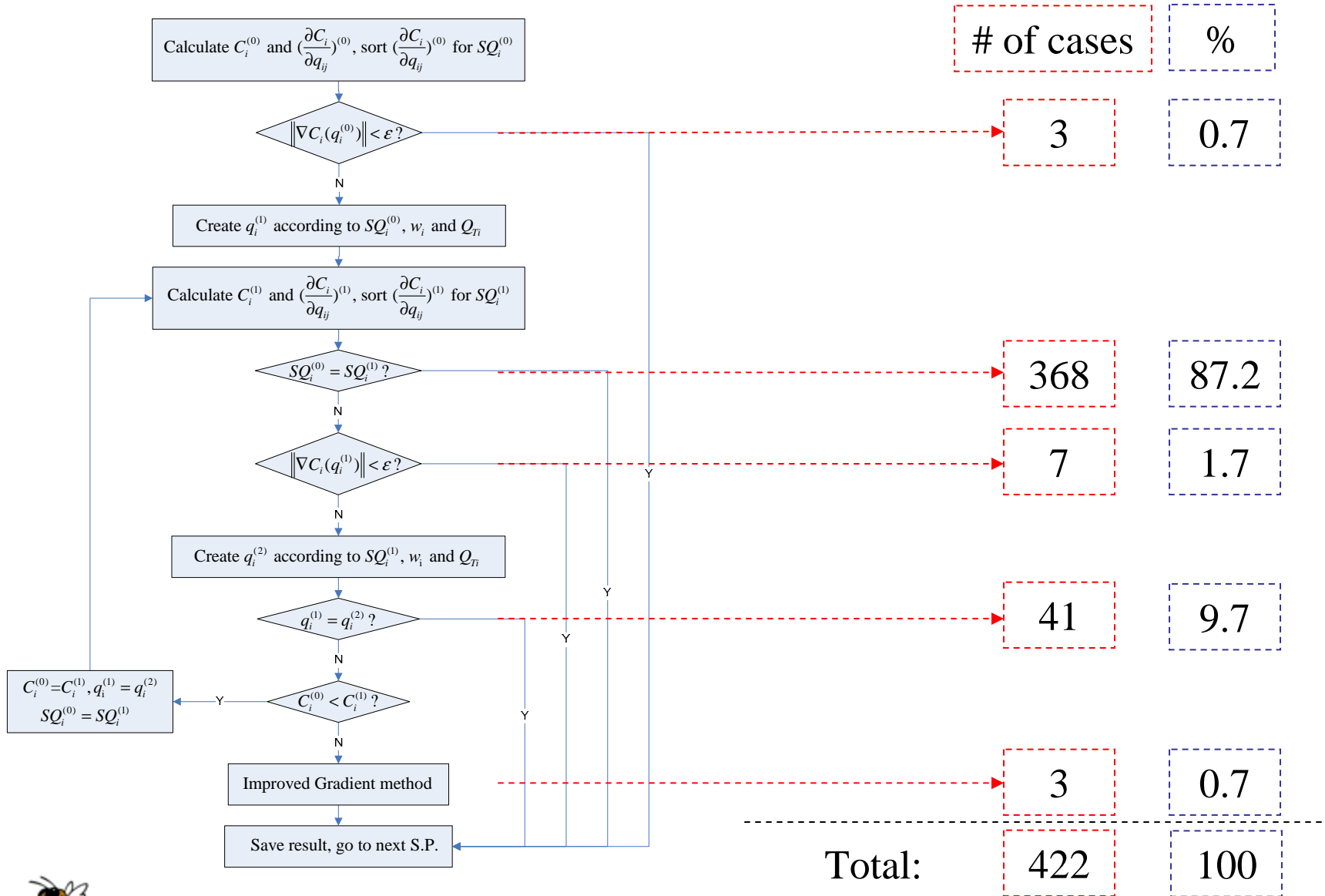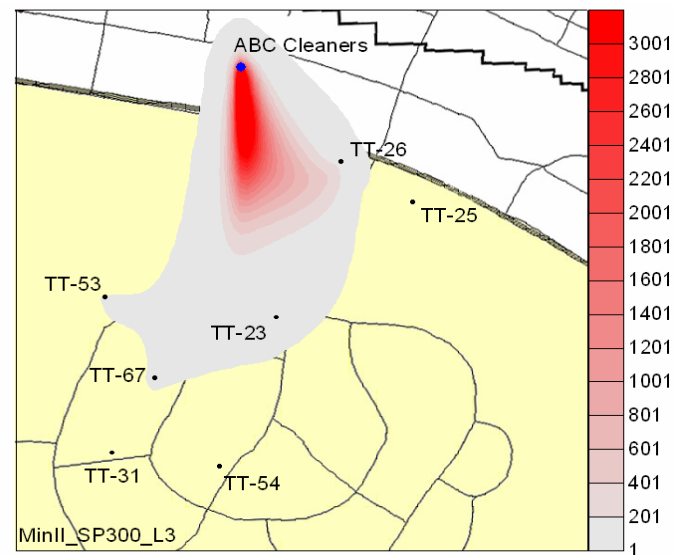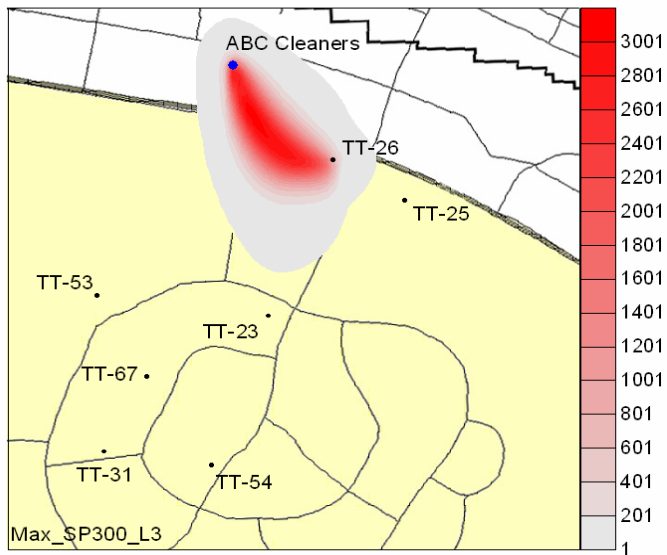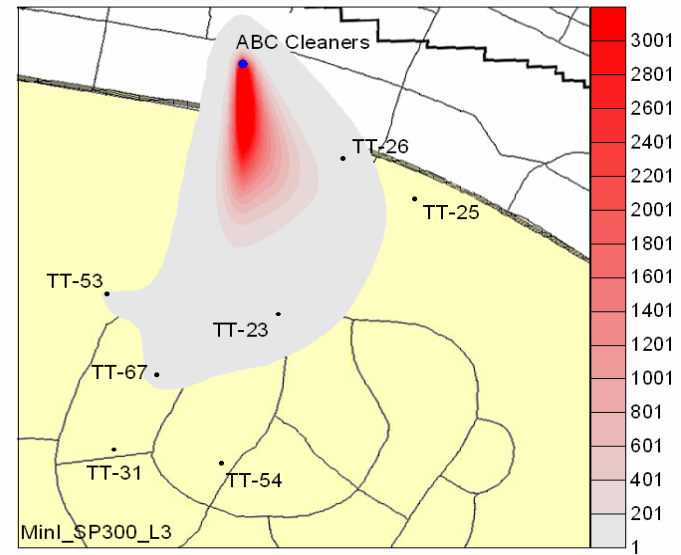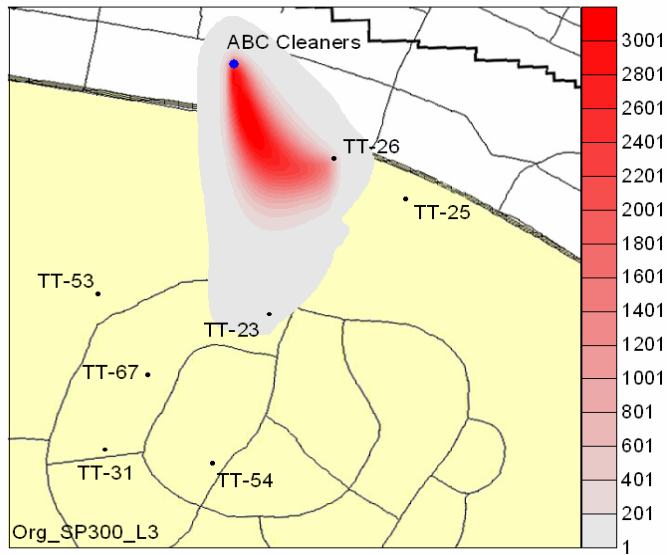
PSOpS Algorithm
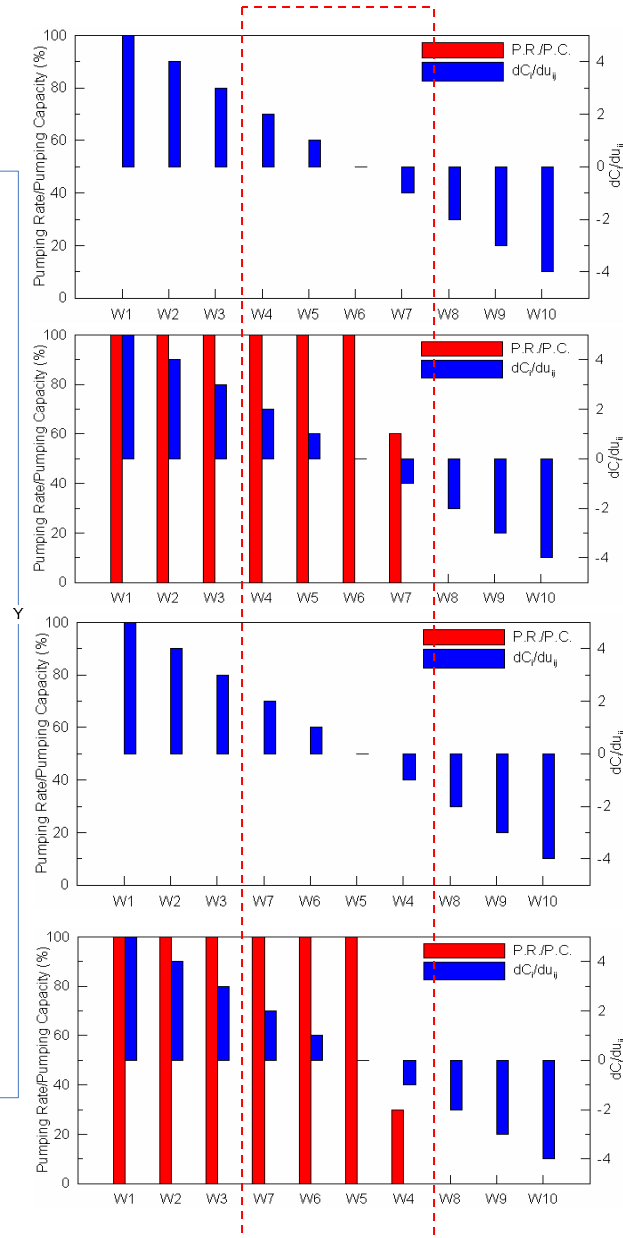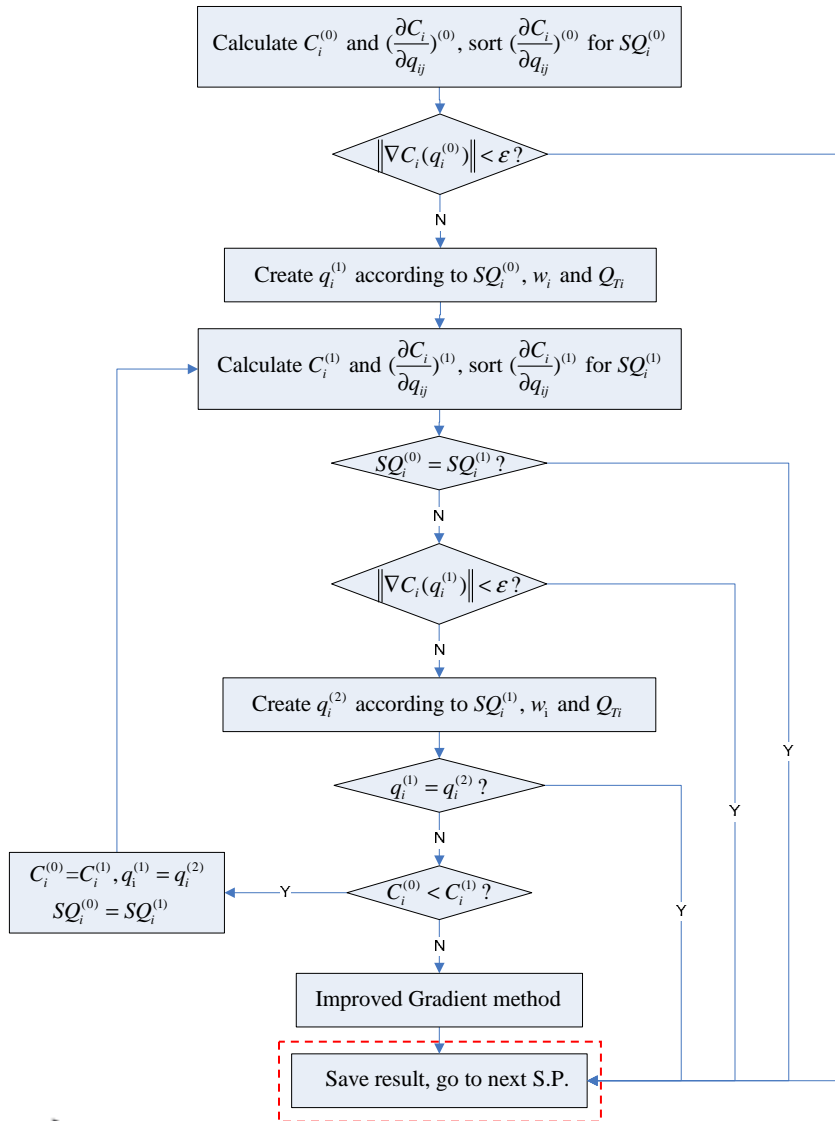
At the end of each SP, head and conc. are saved and chosen to be the starting points for simulation of the next SP. Thus we avoid repeating the simulation from SP1 again and this saves computation cost.

Example of a PSOpS Process

Process Step	# of cases	%
Calculate $C_i^{(0)}$ and $(\frac{\partial C_i}{\partial q_{ij}})^{(0)}$, sort $(\frac{\partial C_i}{\partial q_{ij}})^{(0)}$ for $SQ_i^{(0)}$		
$\left\|\nabla C_i(q_i^{(0)})\right\| < \varepsilon$?	3	0.7
Create $q_i^{(1)}$ according to $SQ_i^{(0)}$, w_i and Q_{Ti}		
Calculate $C_i^{(1)}$ and $(\frac{\partial C_i}{\partial q_{ij}})^{(1)}$, sort $(\frac{\partial C_i}{\partial q_{ij}})^{(1)}$ for $SQ_i^{(1)}$		
$SQ_i^{(0)} = SQ_i^{(1)}$?	368	87.2
$\left\|\nabla C_i(q_i^{(1)})\right\| < \varepsilon$?	7	1.7
Create $q_i^{(2)}$ according to $SQ_i^{(1)}$, w_i and Q_{Ti}		
$q_i^{(1)} = q_i^{(2)}$?	41	9.7
$C_i^{(0)} = C_i^{(1)}, q_i^{(1)} = q_i^{(2)}$, $SQ_i^{(0)} = SQ_i^{(1)}$		
$C_i^{(0)} < C_i^{(1)}$?		
Improved Gradient method	3	0.7
Save result, go to next S.P.		
Total:	422	100

PCE Distribution under Different Schedules

PCE Conc. under Different Schedules
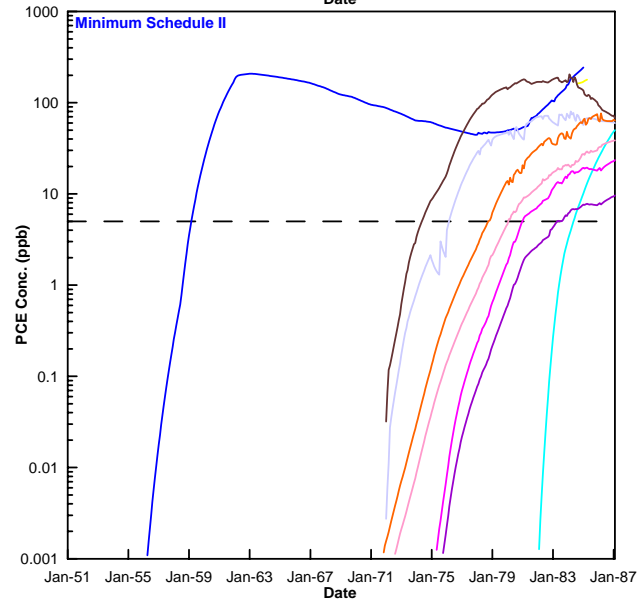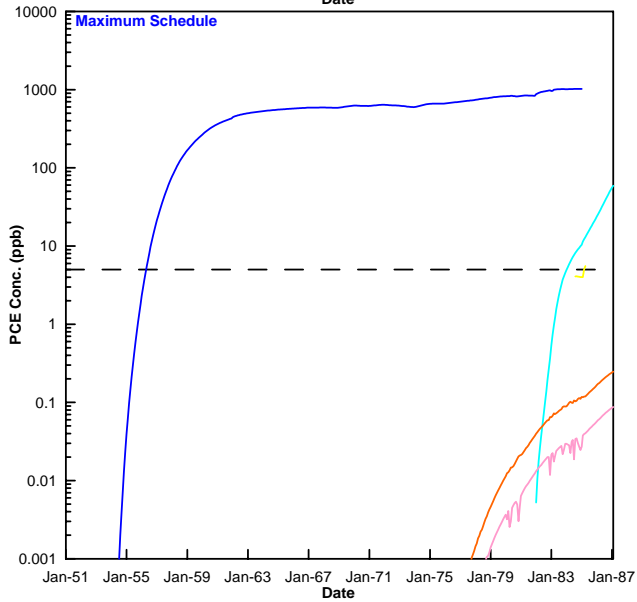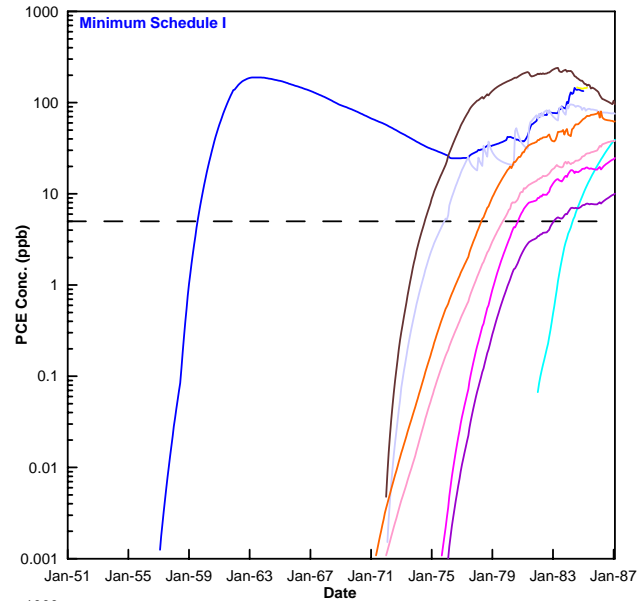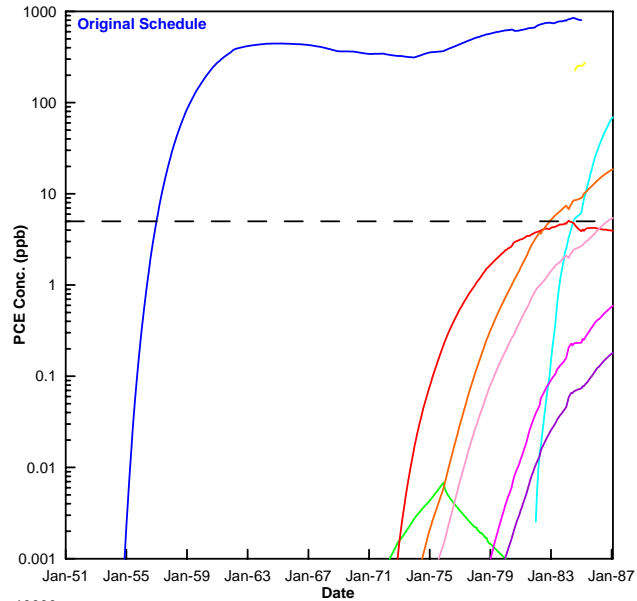
PCE Conc. in WTP and PR in TT-26
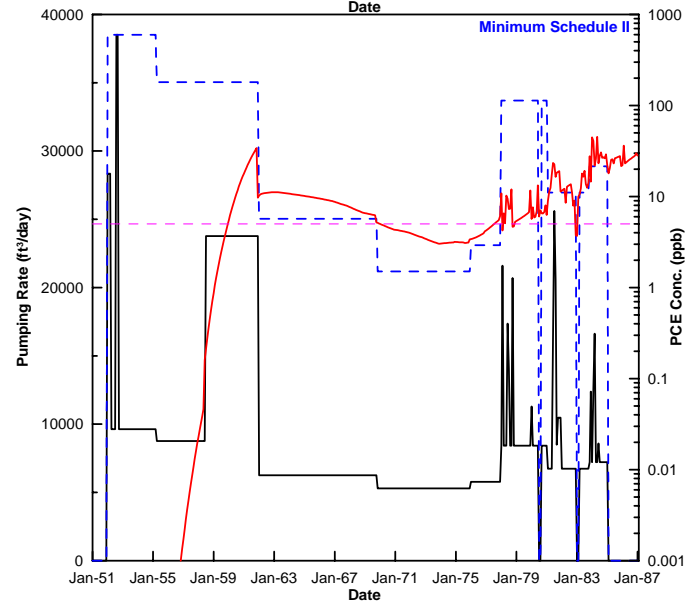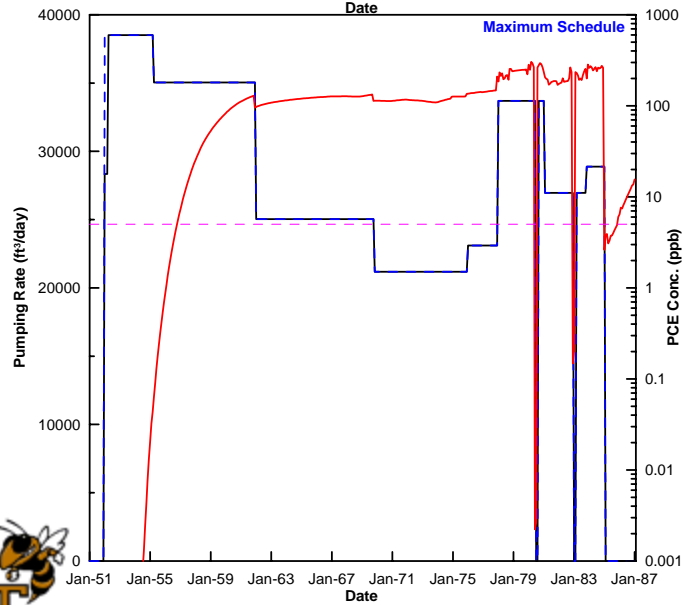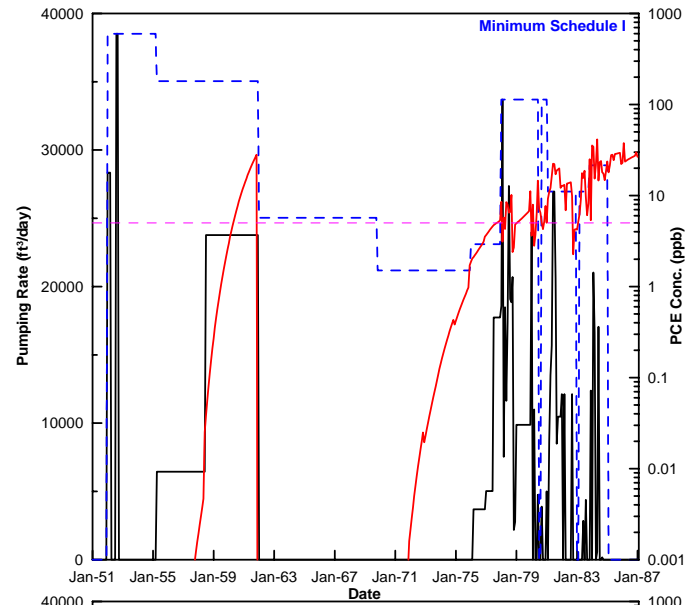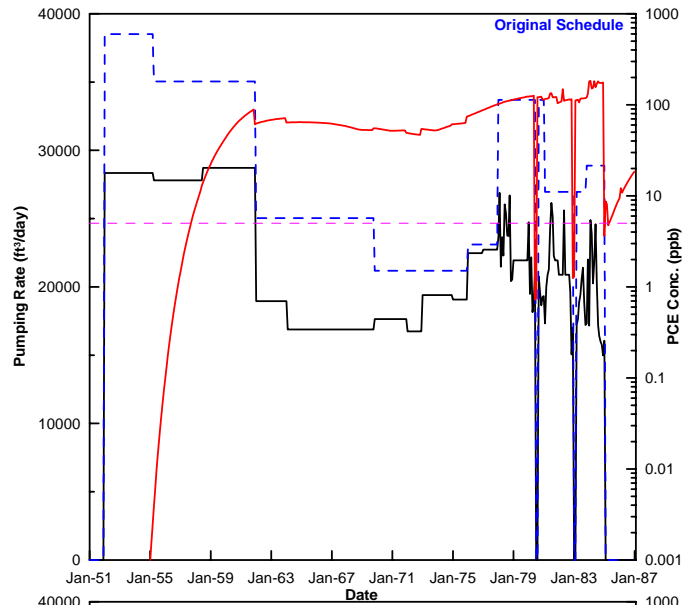
Evaluation Results
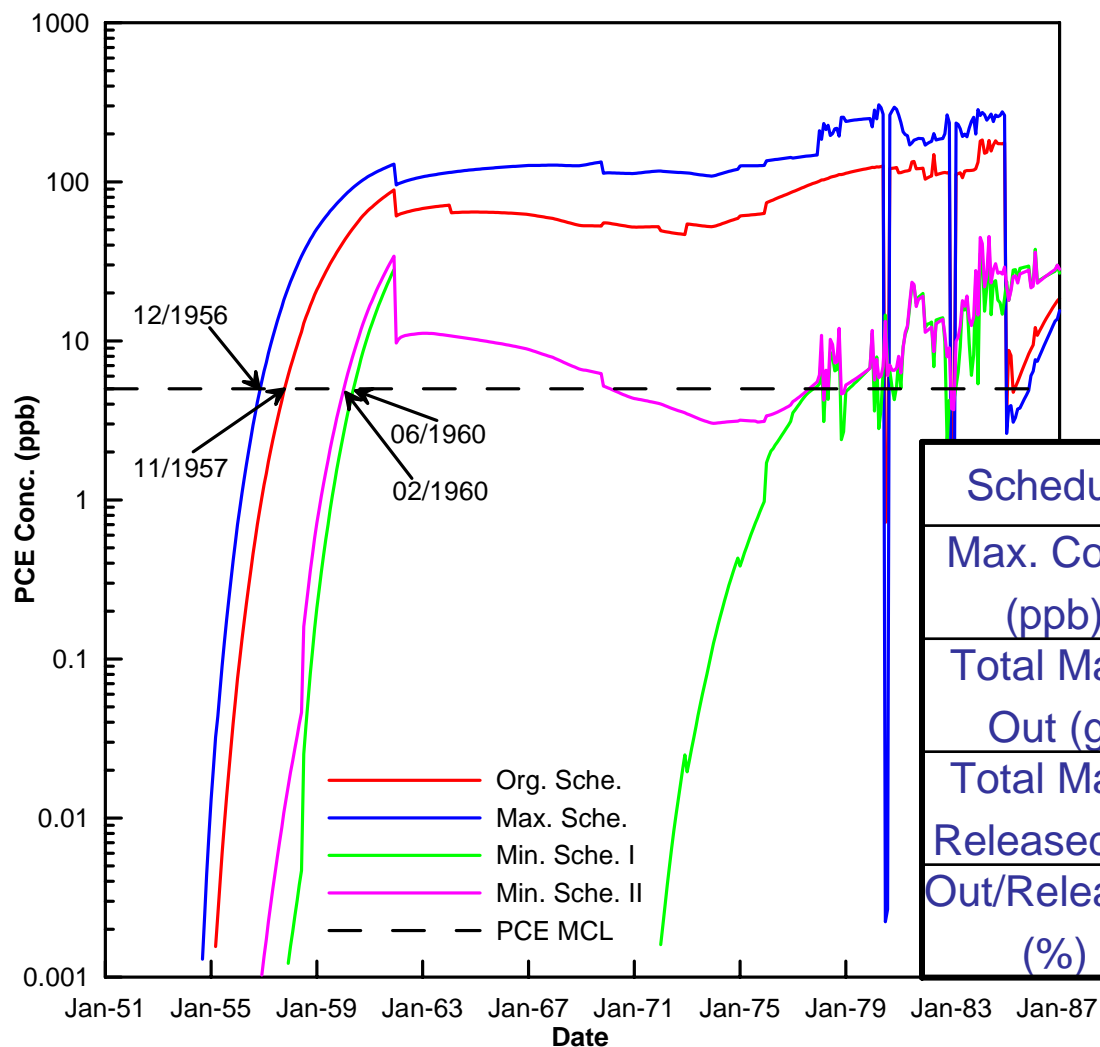
Schedule	Org.	Max.	Min. I	Min. II
Max. Conc. (ppb)	183.04	304.66	41.36	45.31
Total Mass Out (g)	2.45E6	4.59E6	1.98E5	3.41E5
Total Mass Released (g)	1.40E7	1.40E7	1.40E7	1.40E7
Out/Released (%)	17.50	32.78	1.41	2.44

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