Optimization of Large Scale Subsurface Environmental Impacts: Optimal Remedial Design

Deschaine, L. M., Katyal, A. A., and Pintér, J. D.

Conference on Accelerating Site Closeout, Improving Performance, and Reducing Costs through Optimization, June 15th – 17th, 2004, Dallas Texas.

Why Optimize Remediation Designs?

- Groundwater plume migration management and remediation treatment is a costly and time-consuming process.
- Life cycle cost savings.
  - Up to $72.6M to $100M.
- More effective designs.
  - TCE remediation [8 vs. 29 yrs, 40% cheaper].

These results do not indicate that the original designs were necessarily “bad”, just that it is very difficult to develop optimal remediation schemes without optimization tools.

Key Aspects

- Designing of efficient aquifer management solutions involves:
  - The use of simulation models to predict processes such as subsurface fluid movement and contaminant transport.
  - Optimization algorithms to determine best design to meet objectives.

Robust Environmental Simulators

- SA_MAPS
  - Stream - Aquifer Management and Planning Simulator
- BioFT3D/MINTEQ
  - Flow and Transport in the Saturated and Unsaturated Zones in 2 or 3 Dimensions
- BIOSLURP
  - Multiphase Hydrocarbon Vacuum Enhanced Recovery & Transport
- MOFAT & NAPL 2D/3D
  - Multiphase Flow and Transport of Multicomponent Organic Liquids

For additional information, see rasint.com & georgepinder.com

Optimal Estimation of Subsurface Conditions

- Subsurface state estimates are uncertain.
- Optimal estimation is achieved via:
  - Physics models + data models + geostatistics + information fusing / signal processing algorithms (Kalman filter or genetic programming).

Challenge is to match the reduction in uncertainty with the project objectives and cost of information.

General Mathematical Statement

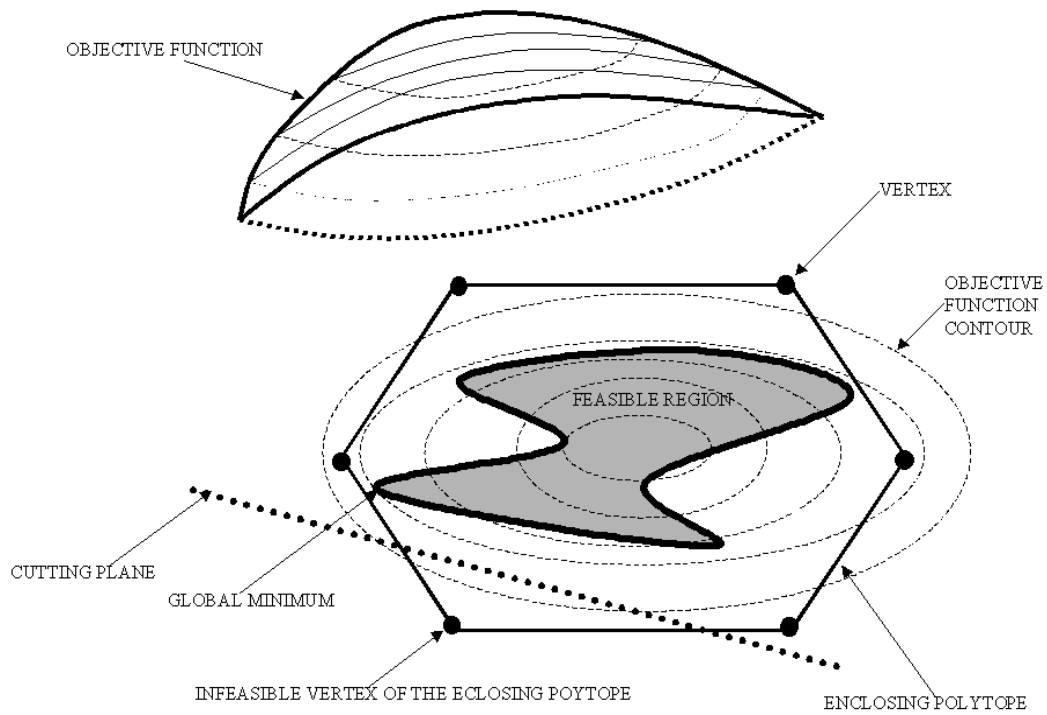
- Minimize f(x); the cost of the action
- Subject to:
  - $x \in D$; the constraints on the solution
- Seemingly simple, it is often difficult or impossible to do this completely.
- Function calls to the objective are very expensive, hours /weeks per call.

Robust Global Optimization Algorithms

- Outer Approximation Method
  - Karatzas & Pinder
- Lipschitz Global Optimization
  - Pintér
- VT_Direct
  - Watson/He (Virginia Tech)

For additional information, see www.informs.org & www.dal.ca/~jdpinter/ & http://www.cs.vt.edu/info/people/vitae/Watson.html

The Concept of the Outer Approximation Method.



Developed by Dr. Tuy mid 1960's, published in Vietnam, translated to Russian, then to English, extended by Drs. Karatzas and Pinder – RCGRD.

Lipschitz Global Optimization

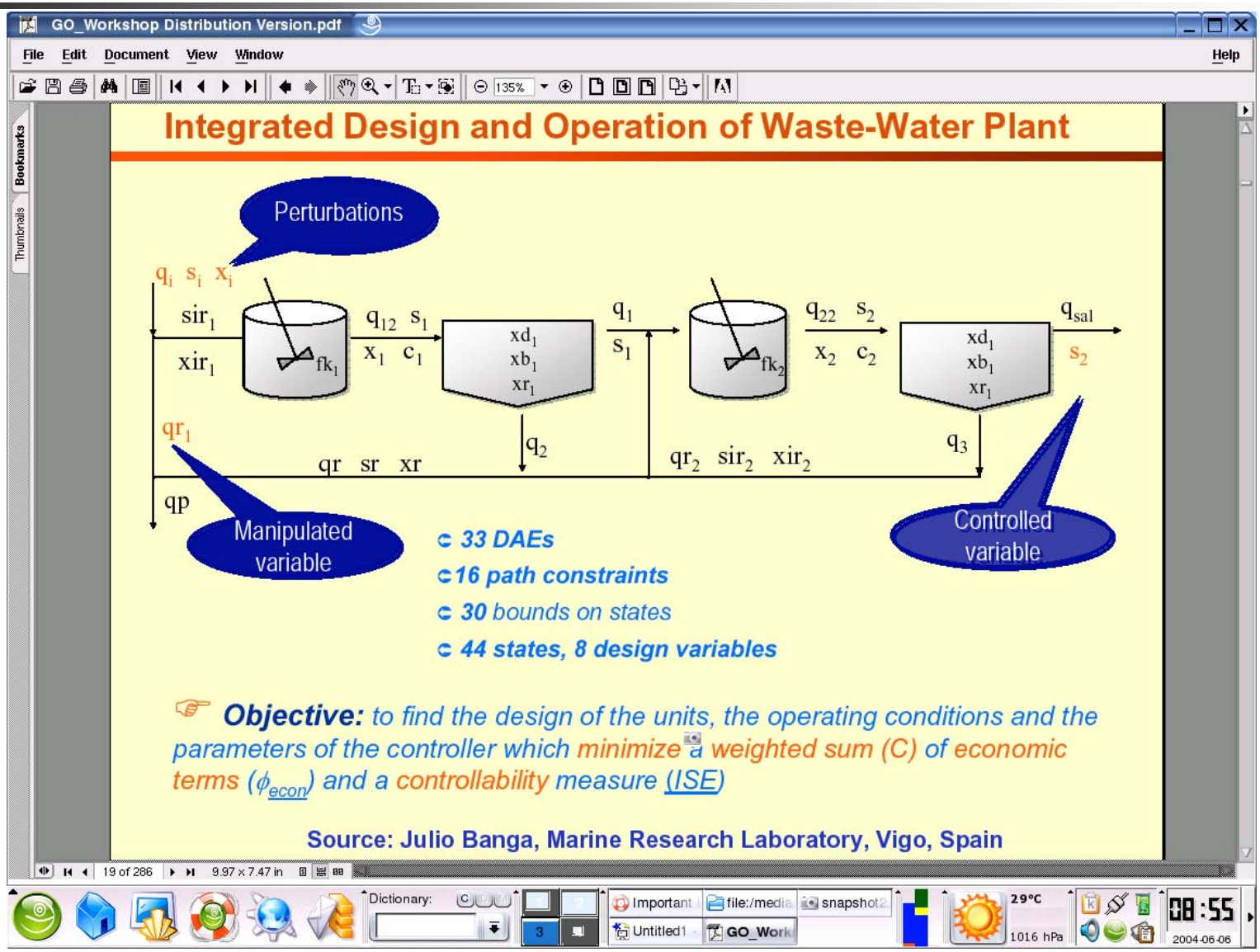
- Globally convergent methods:
  - continuous branch-and-bound (adaptive partition & search)
  - global adaptive randomized search
  - multi-start based adaptive random search
- Locally convergent methods:
  - exact penalty function approach

Available as callable object from Fortran and C/C++, linked with Mathematica, Excel, GAMS, peer-reviewed.

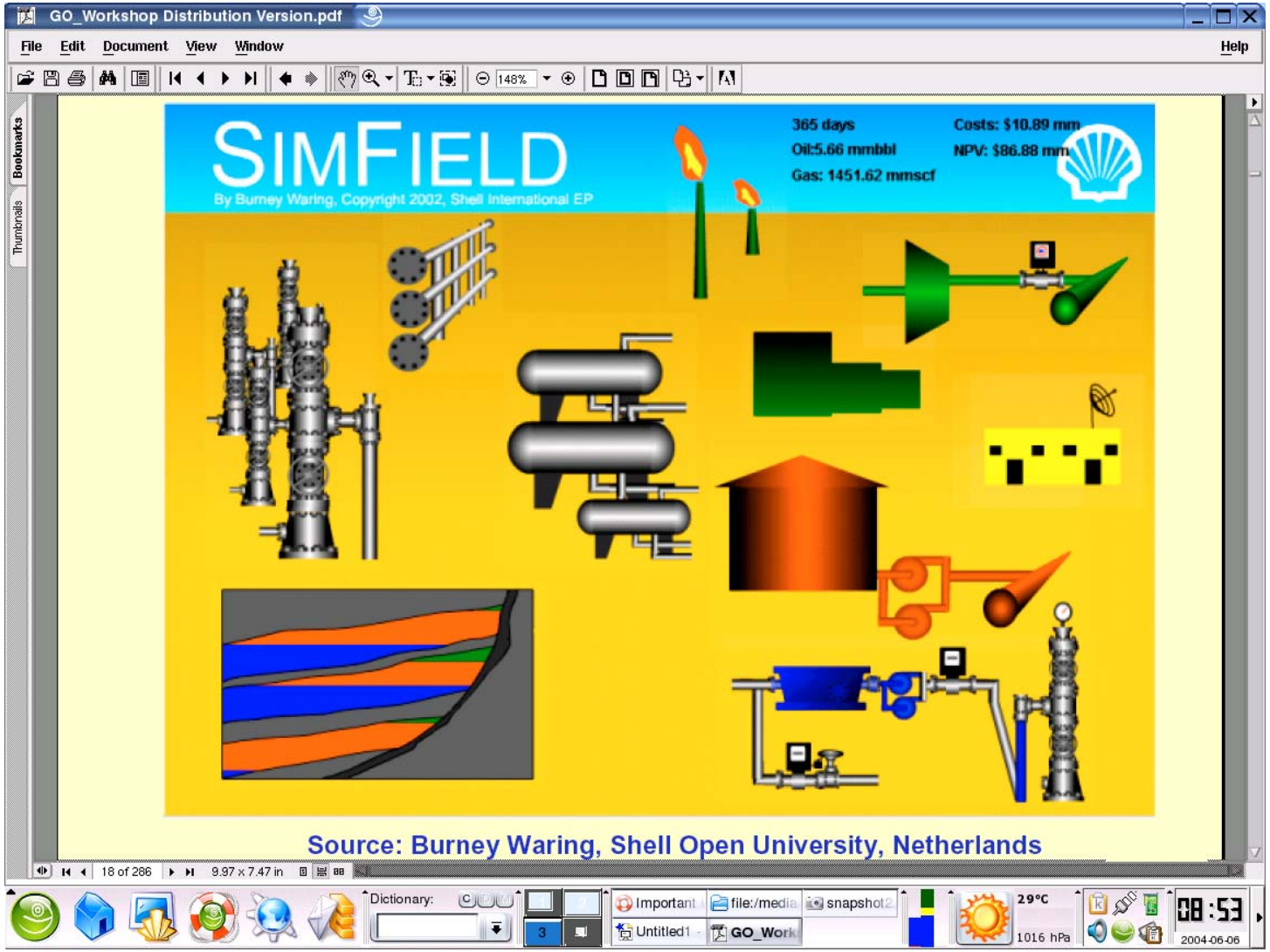
The Optimal Remediation Design Process

- The treatment plant and/or in-situ remediation system consists of:
  - Installation costs
  - Operations costs
- Solution must meet the design objectives:
  - Point or area of compliance
  - Concentration to be met
  - Desired time to meet the compliance
- Solution chosen:
  - Least cost technology implementation that meets the design objectives

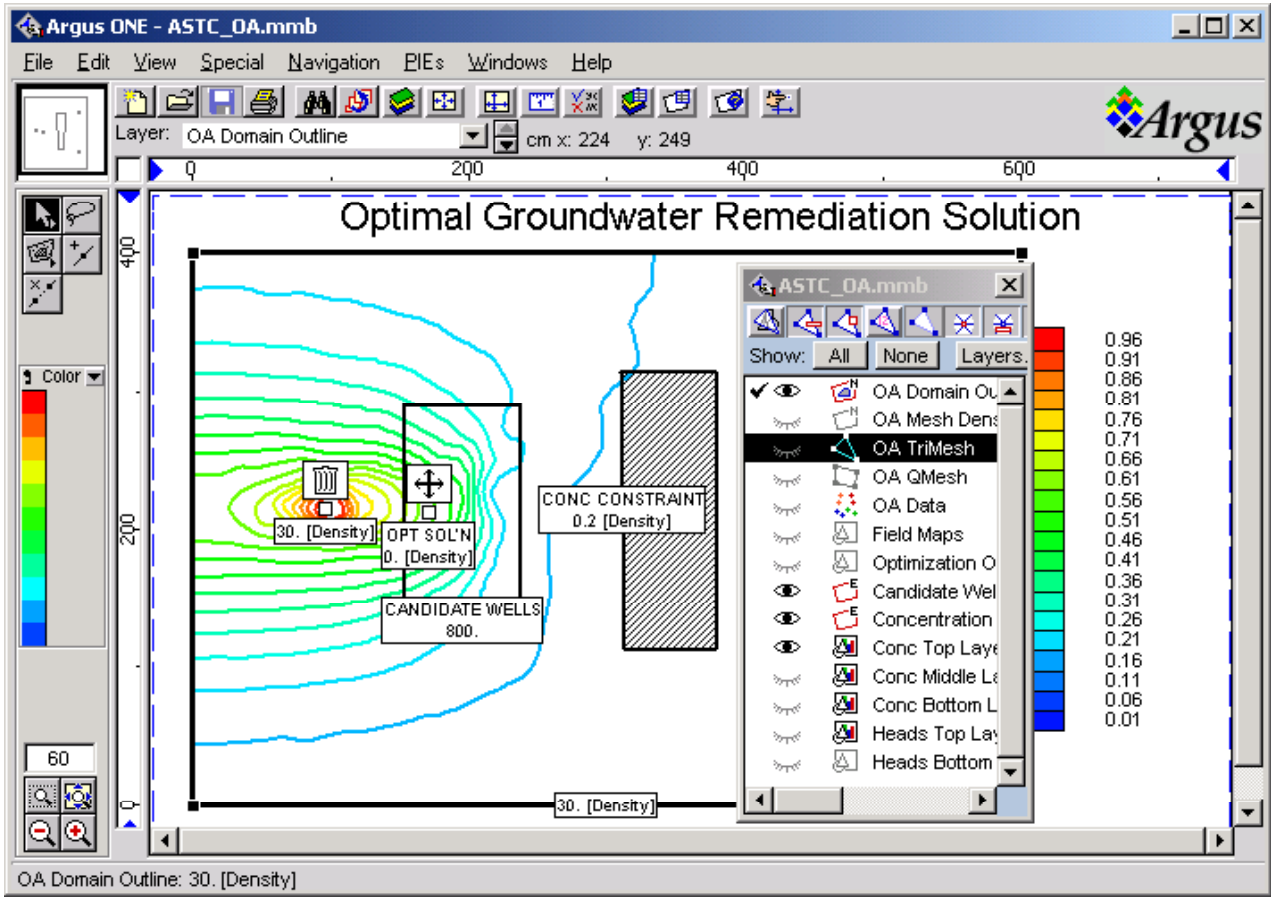
Simple Illustration of Challenge: Above Ground Treatment Plant



Simple Illustration of Challenge: Oil Field Process Optimization



Simple Illustration of Challenge: Groundwater Pollution

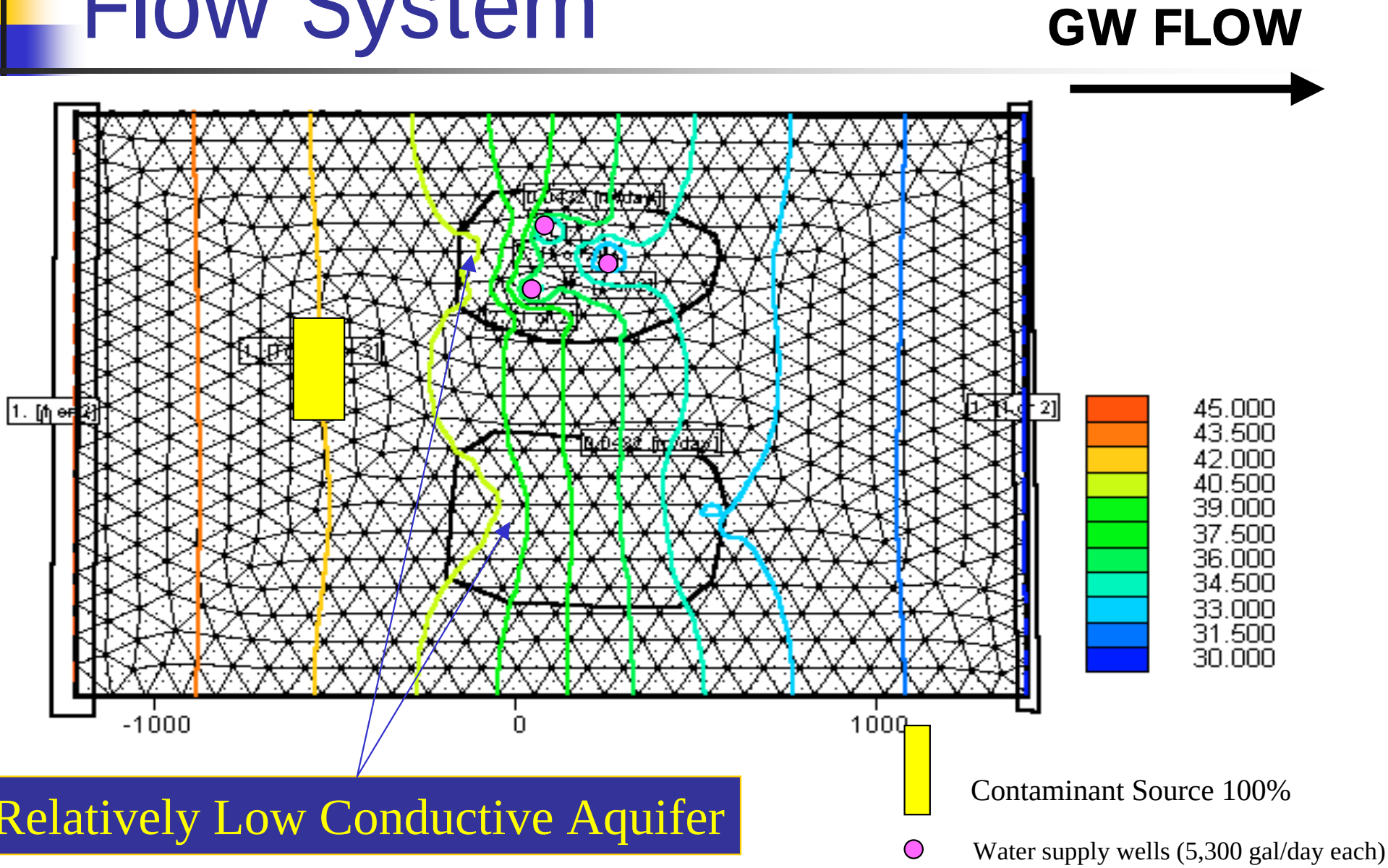


A below-ground wastewater treatment plant process

Detailed Example Subsurface Remediation

- Source located in drinking water aquifer
- Point of compliance located between the source as some low flow water supply wells.
- Stakeholders want to know the likely costs for various risk-based clean-up standards to help make an informed decision.

Detailed Example: Flow System



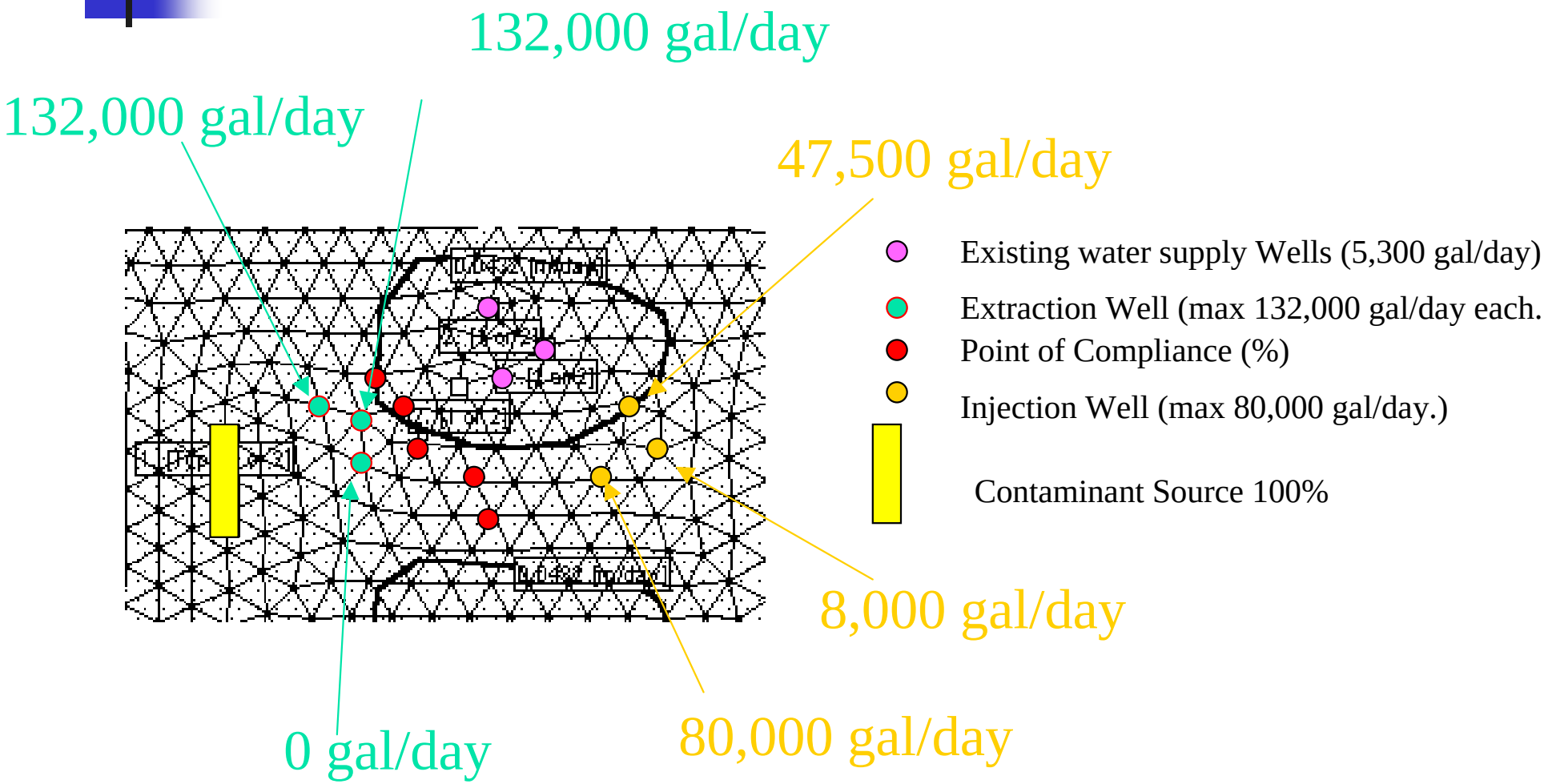
Relatively Low Conductive Aquifer

Inputs for Optimization

- Source location [point, area].
- Source strength [fixed, variable].
- Area where treatment can occur.
- Point or area of compliance.
- Treatment technology.
- Time for remediation to be complete.
- Cost per well [$].
- Cost to operate and monitor system [$/yr].

Ponder: Is it better to pump a little water at high concentration or a lot of water at low concentration...?

Detailed Example: One Optimal Solution



One Optimal Solution for a Specific Clean-up Level. Note that water reinjection can occur to conserve this natural resource.

Detailed Groundwater Remediation Solution Output

Reduction in Source Strength Needed @ POC	Solution	Cost
Greater than 80%	TI Zone	Negotiated
65% to 80%	Active Remediation	$200K to $900K
Less than 65%	MNA	$150K

Provides framework to achieve consensus stakeholder approved solutions

Output

- Best design basis for the remediation system.
  - Location, injection / extraction rates.
- Optimal life cycle cost of remediation.
- Sensitivity graphs:
  - Clean-up technology vs. Compliance point locations vs. Compliance concentration levels vs. Costs.
- Excellent tool for stakeholder groups.
  - If conflicting design constraints are added, it will tell you that feasible solution does not exist.

Provides a tool to work towards feasible solutions

Technology Extensions

- The example shows optimization of groundwater pump and treat system.
- Extensions include capability to optimize:
  - Bioairsparging systems.
  - Design optimization of in-situ redox zones.
  - Separate phase [LNAPL, DNAPL] product recovery.
  - Soil vapor extraction systems.
  - Monitored natural attenuation enhancements, etc.

Extensions comprise of hooking the right combinations of simulator(s) and optimizer(s) to the specific challenge. Genetic programming used when fused physics-data models unavailable.

Site-Wide (Global) Optimization

- Links:
  - Plume finding
  - Plume remediation
  - Technical impracticability
  - Long-term monitoring
- Into a single comprehensive analysis framework

See: Deschaine, L. M., Simulation and Optimization of Large Scale Subsurface Environmental Impacts; Investigations, Remedial Design and Long Term Monitoring. Journal of "Mathematical Machines and Systems", National Academy of Sciences of Ukraine, Kiev. No 3, 4. 2003. Pages 201-218.

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D4 Optimal Answer (1)

Site Wide Optimization: Larry M. Deschaine, PE
Chalmers University of Technology, Goteborg, Sweden, Department of Physics
[Ph.D. Dissertation, 2002]

Source Area	X-coord	Y-coord	Optimal Answer (1)	Mgt. Priority: 1=Required; 0=Possible; -1=Exclude	Analyst's Solution attempt; link to autoSolution Generator	Technology Description(1)	Cost Estimate Range (2) Low	Med.	High
SWMU 1	2500	1000	1	0		MNA	$250,000	$300,000	$350,000
SWMU 1	2500	1000	1	0		Cap/Remove	$750,000	$1,000,000	$1,250,000
SWMU 1	2500	1000	0	0		Treat	$2,000,000	$2,500,000	$3,000,000
SWMU 2	3750	500	1	0		MNA	$100,000	$150,000	$200,000
SWMU 2	3750	500	0	0		Cap/Remove	$500,000	$600,000	$700,000
SWMU 2	3705	500	0	0		Treat	$1,000,000	$2,000,000	$2,500,000
SWMU 3	4000	2000	1	0		MNA	$500,000	$600,000	$650,000
SWMU 3	4000	2000	0	0		Cap/Remove	$3,000,000	$3,500,000	$4,000,000
SWMU 3	4000	2000	0	-1		Treat	$10,000,000	$12,000,000	$20,000,000
SWMU 4	4500	3250	1	1		MNA	$300,000	$400,000	$450,000

Optimal answer: $2,450,000

1. The optimal answer is for the site-wide system, the technologies compete for a place on the solution team.
2. Treatment is any of the processes that remove source material or reduce mass flux loading
3. The cost estimate is either deterministic or stochastic as specific by contract vehicles / professional judgment

All the constraints are located to the right
1) Annual min. & max funding
2) Annual max mass-flux discharge
3) Other constraints on the solution

Unlimited year planning and Alternativies evaluation

Master Controller / Cost Storage / Environmental Discharge Constraints

Sheet 1 / 3 Default 118% STD Sum=0

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Produces Results

- Blending of physics, mathematics, engineering and construction produces robust solutions to extremely challenging problems.

Record Remediation Wells

Engineer of Record, Larry M. Deschaine, PE

Reference Material

- Pintér, J. D. Global Optimization in Action:Continuous and Lipschitz Optimization: Algorithms, Implementations and Applications. Kluwer Academic Publishers, 478 pp. 1996.
- Huyakorn & Pinder, Computational Methods in Subsurface Flow, Academic Press, 473 pp. 1983.

Acknowledgements

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Thank You...

...for your attention