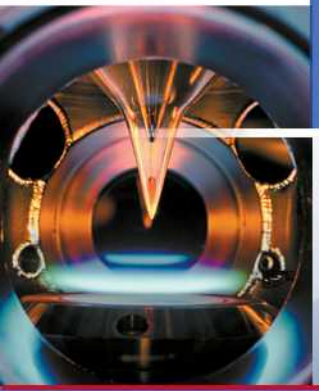
SAND2011-2595C

SANDIA NATIONAL LABORATORIES

Overview of SNL Water Initiative

Mark J. Rigali
Manager, Geochemistry Department
Water Treatment Lead, Sandia Water Initiative
mjrigal@sandia.gov



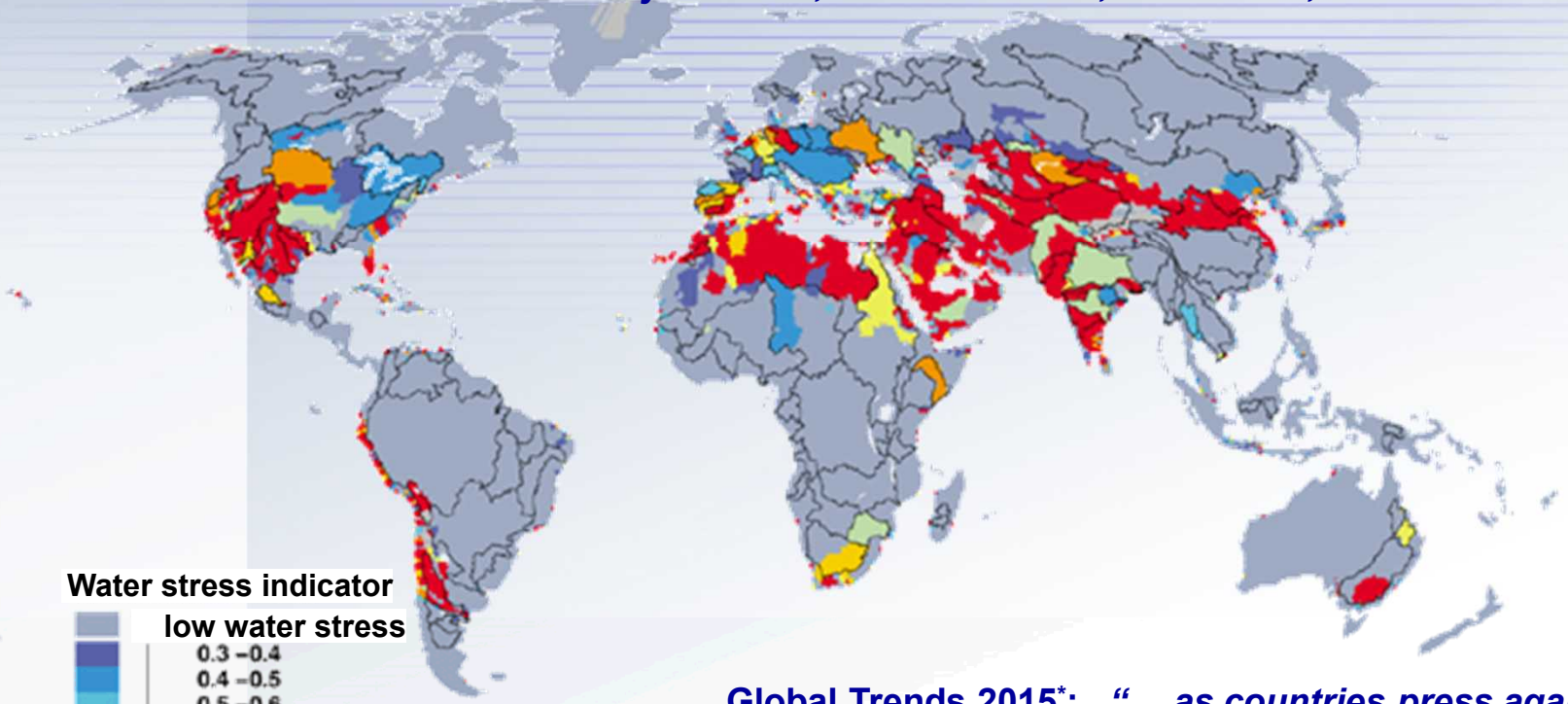
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

Sandia National Laboratories

Water Challenges are Global

Global Trends 2015*:

"By 2015 nearly half the world's population – more than 3 billion people – will live in countries that are water stressed… mostly in Africa, the Middle East, South Asia, and northern China"

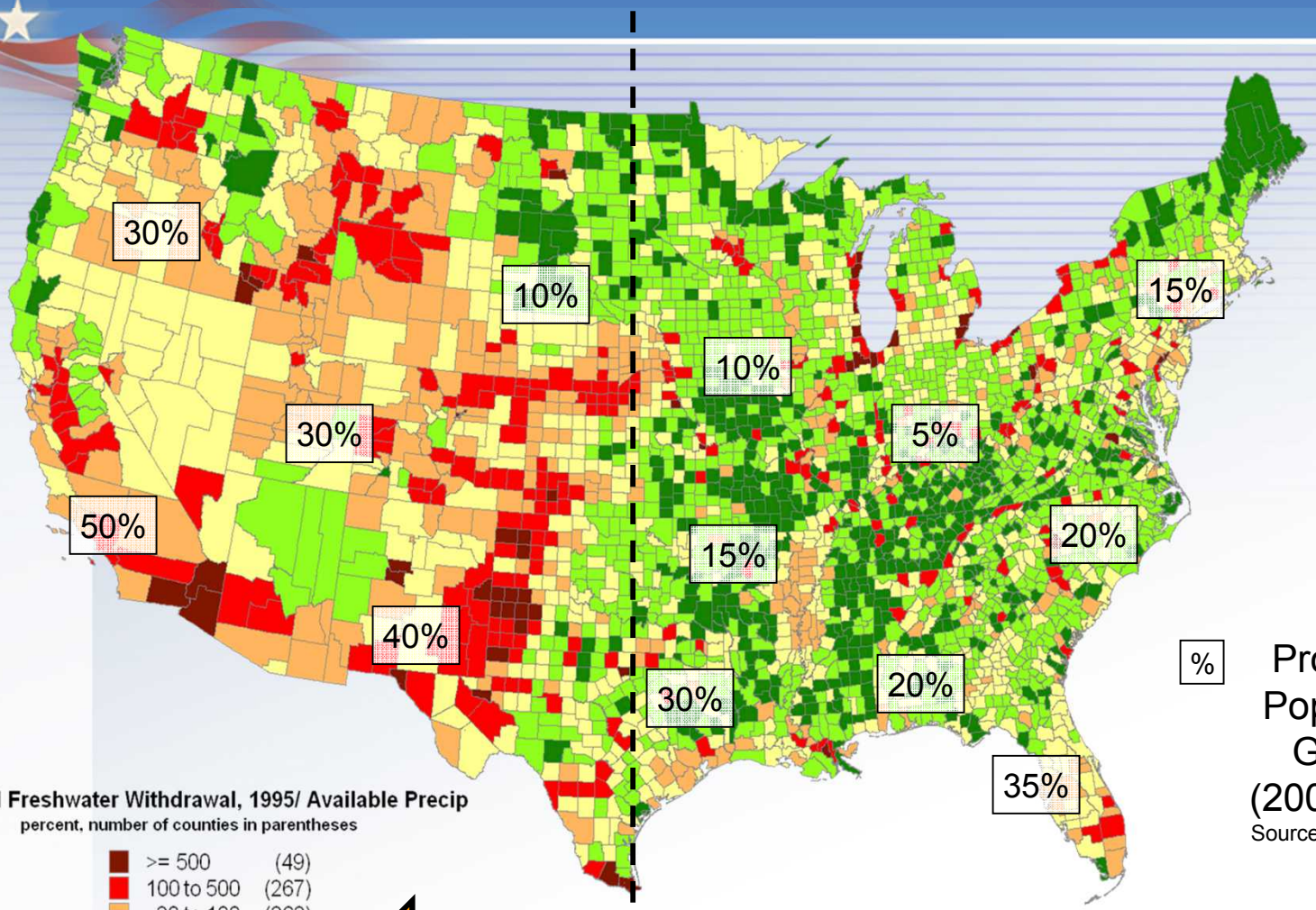


Global Trends 2015*: ***"… as countries press against the limits of available water between now and 2015, the possibility of conflict will increase."***

**Global Trends 2015: A Dialog About the Future with Nongovernmental Experts*, National Intelligence Council, December 2000.

Sandia National Laboratories

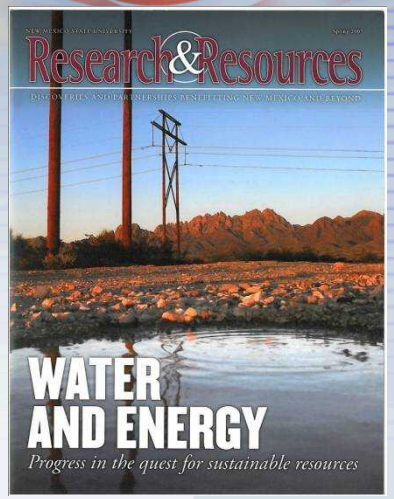
Water Challenges are Nationwide

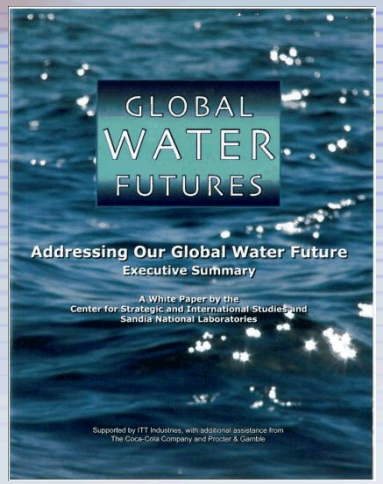


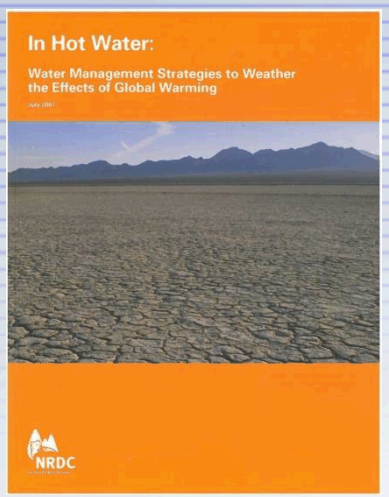
Source: USGS Circular 1200 (Year 1995), EPRI 2003

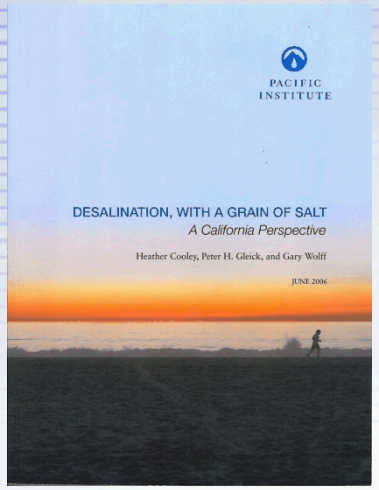
Sandia National Laboratories

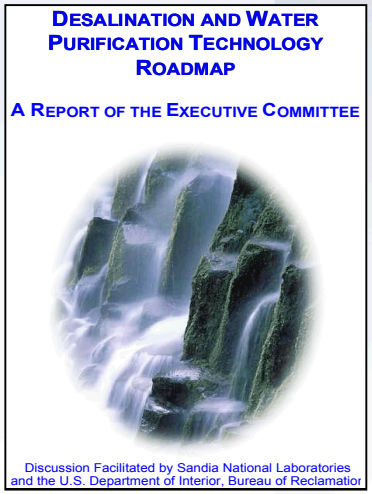
Many documents highlight the issues

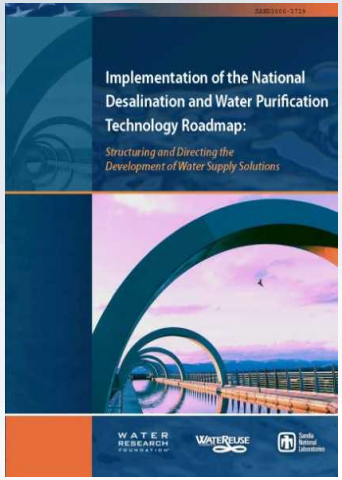


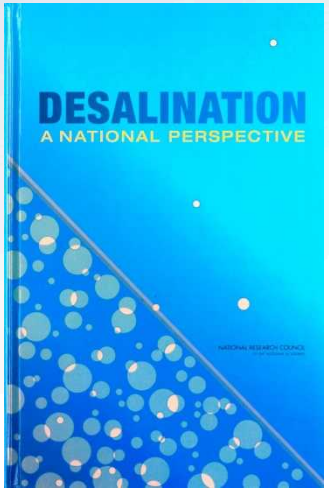


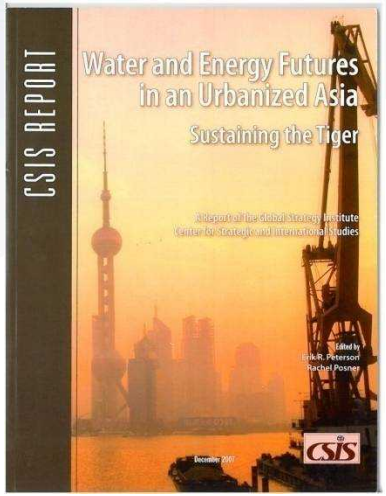


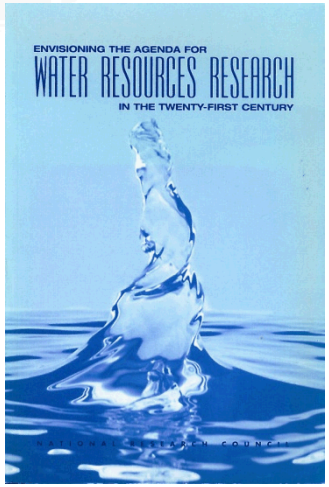










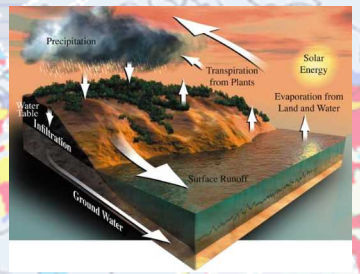


Sandia National Laboratories

Sandia's Water Program

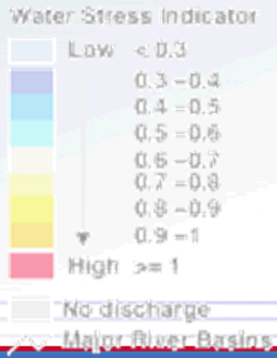
Treatment Technologies

Modeling & Management



Security Systems

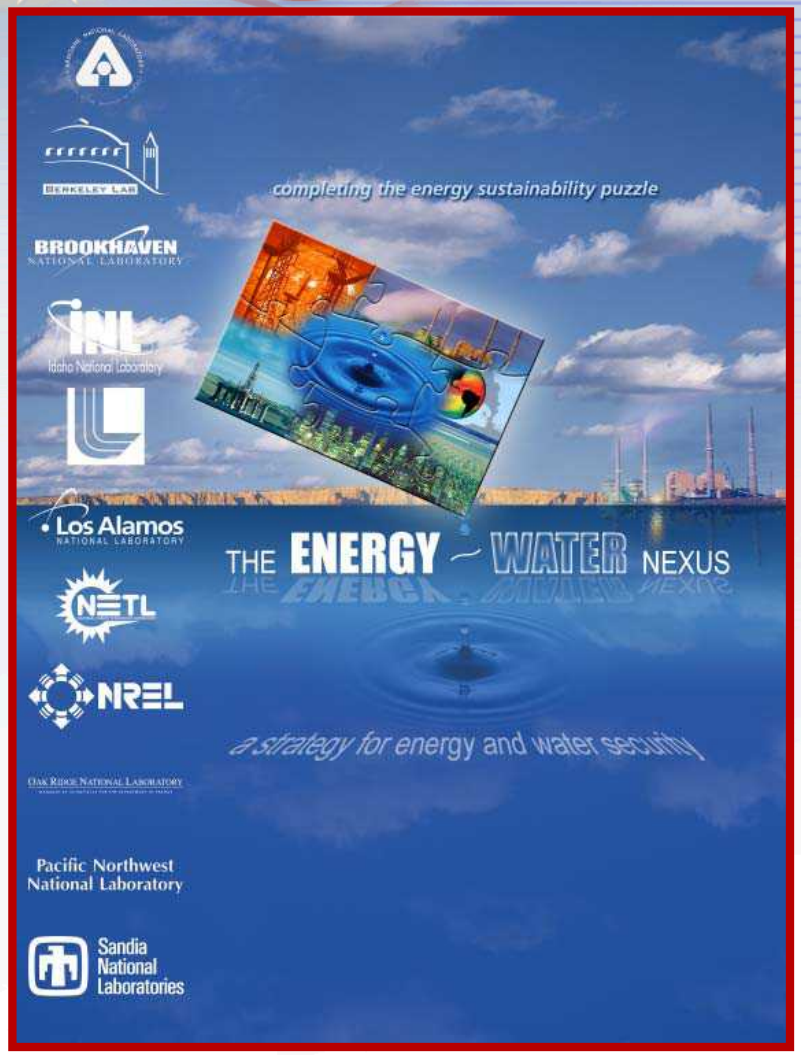
Energy-Water

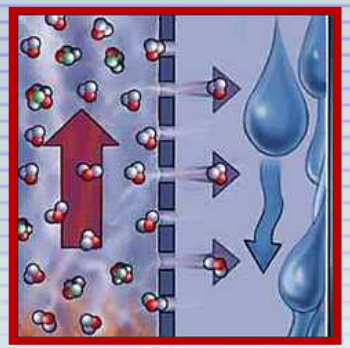


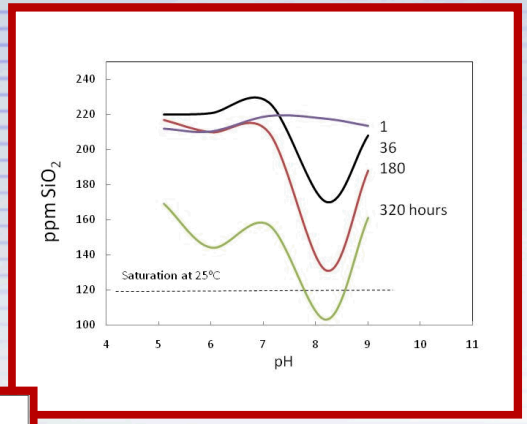
SAFETY · SECURITY · SUSTAINABILITY

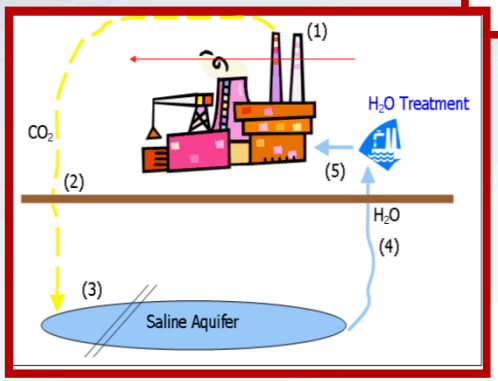
Sandia National Laboratories

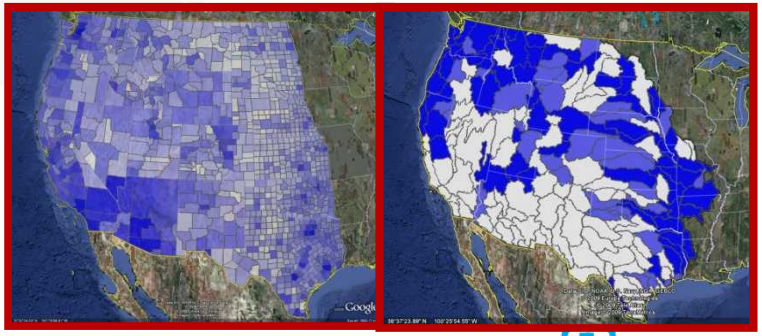
Energy and Water







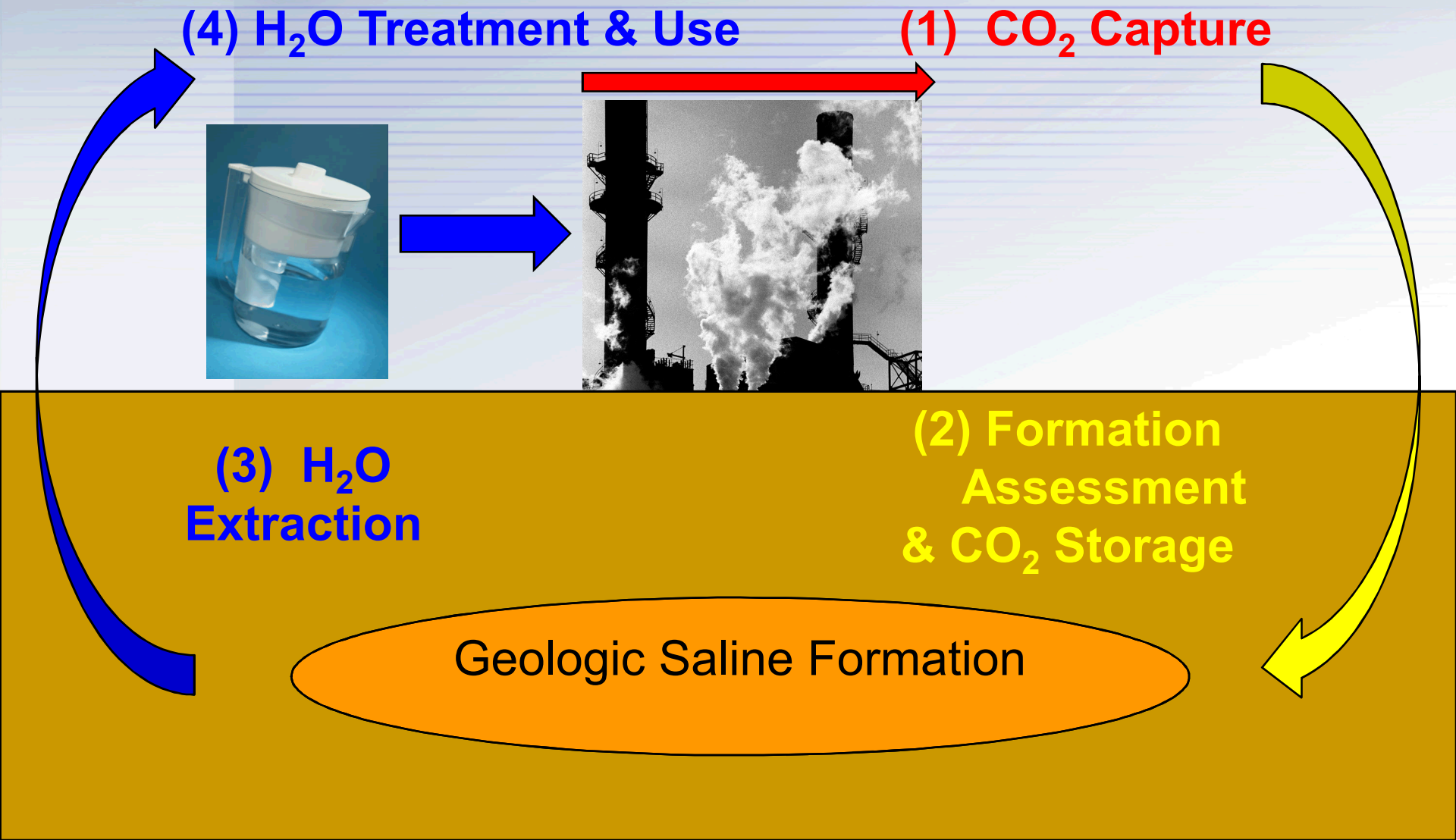




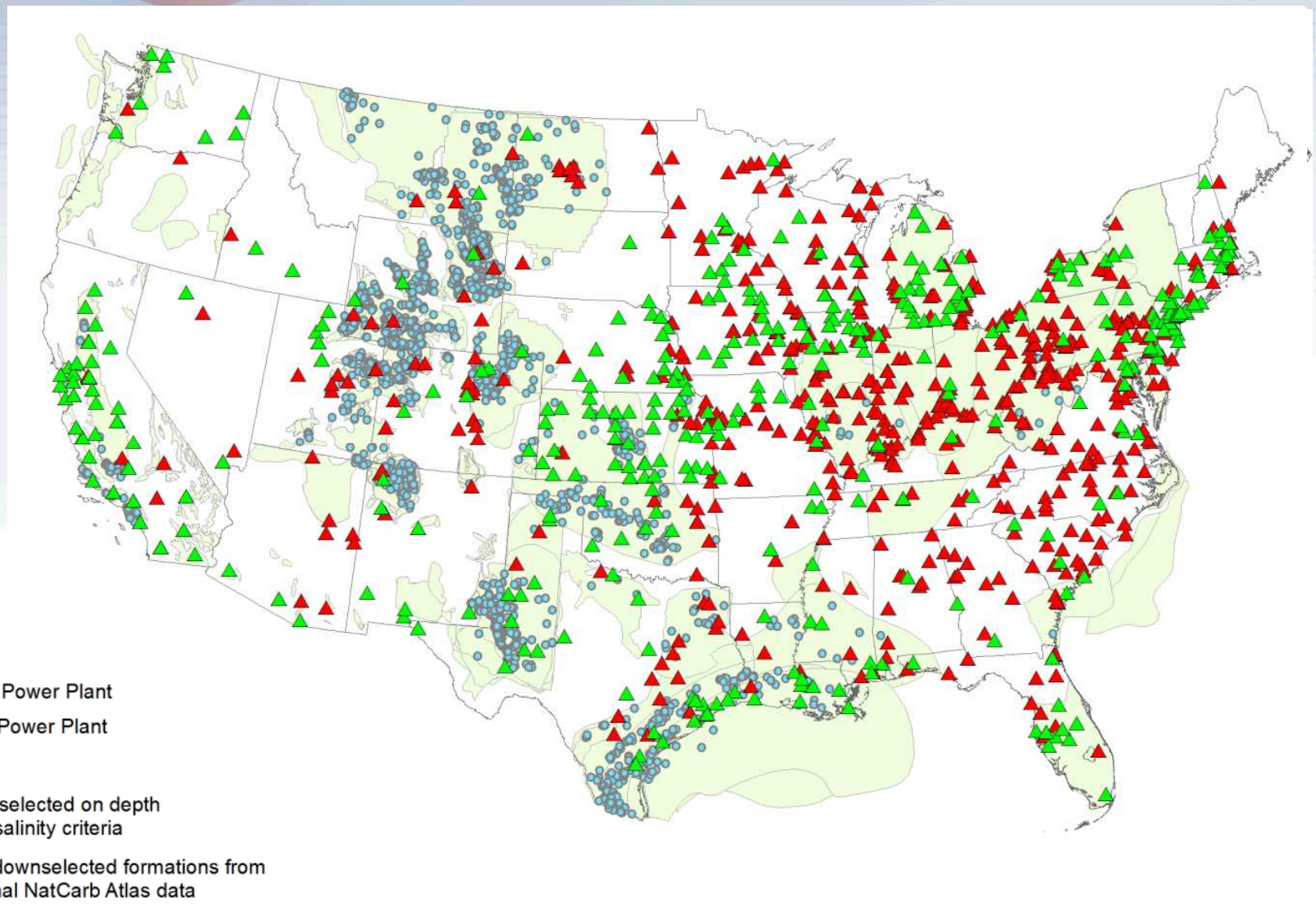
Sandia National Laboratories

Building a Framework for Water, Energy and CO_2 Storage (WECS):

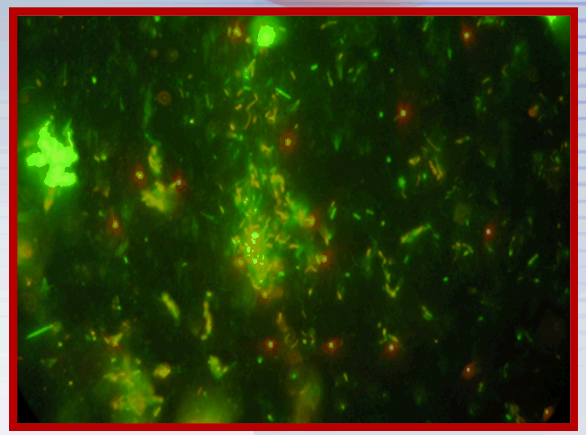
Addressing Uncertainly in the Data



Geological CO_2 Storage Database is Incomplete: *Makes Source/Sink Matching Difficult*



Security Systems

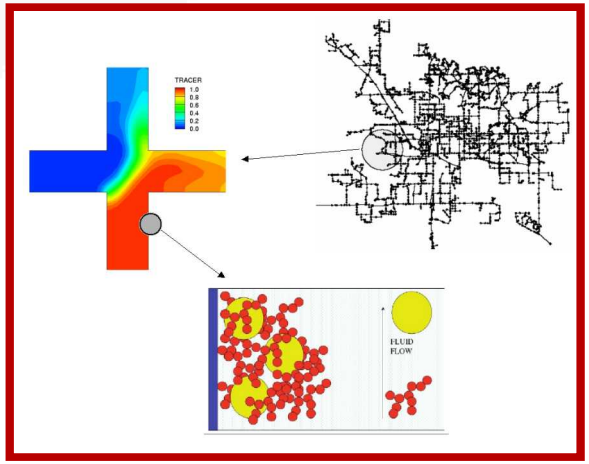


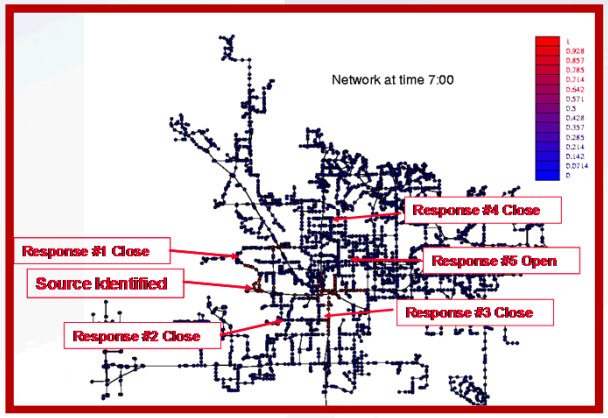
Pathogen Interactions

CANARY Event Detection Software

Lab testing & model validation

Computational Fluid Dynamics



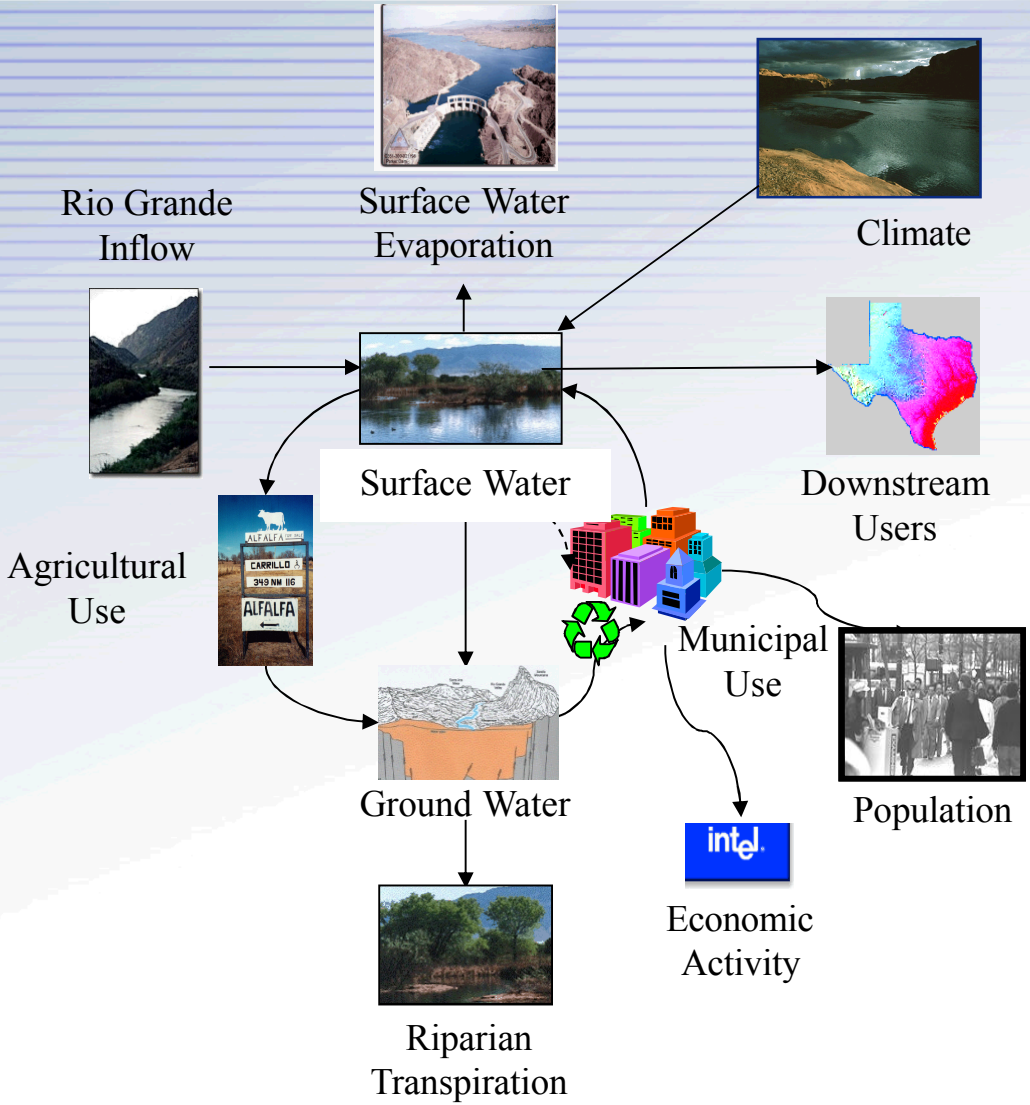


Numerical Algorithms

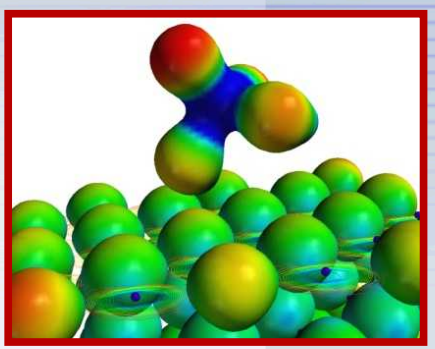
Sandia National Laboratories

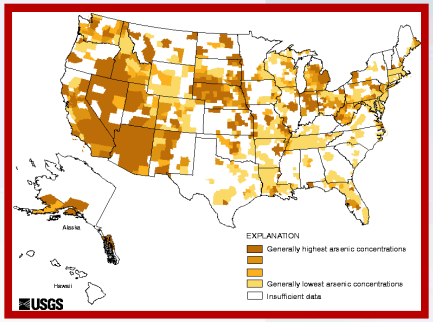
Modeling and Management

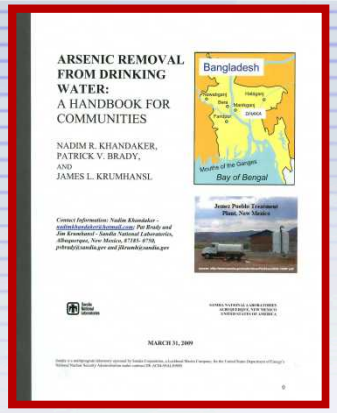
- "Holistic" approach to quantitatively assessing water resource sustainability
- System dynamics provides framework for modeling multiple, interdependent subsystems each varying in time and space
- Focus is on intermediate to long-term interdependencies between resource supply and demand
- Major areas of interest include interdependencies of energy, water, and agricultural sectors since energy and agriculture are large water using sectors



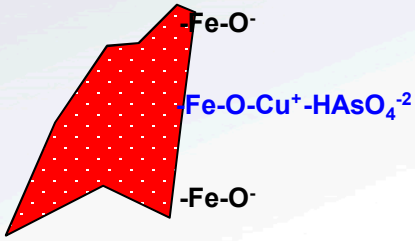
Treatment Technologies: Arsenic





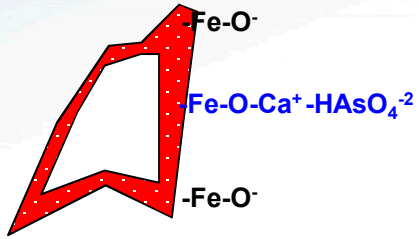


Ex situ



Iron oxide filter media

In situ



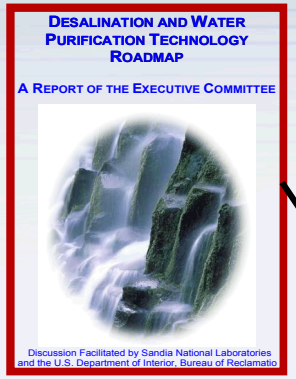
Iron-coated sand aquifer

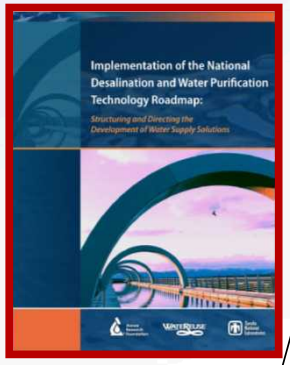
ARSENIC WATER TECHNOLOGY PARTNERSHIP
AwwaRF · SANDIA · WERC

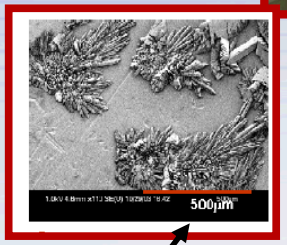
Sandia National Laboratories

Treatment Technologies: Desalination

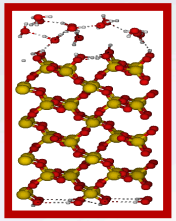
Roadmapping

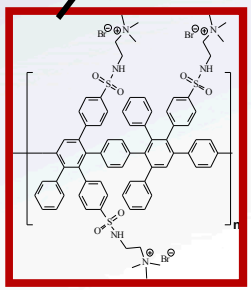






Near-term research



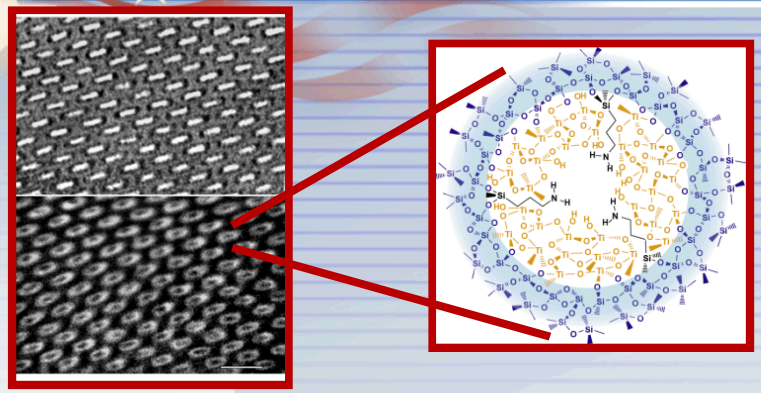


Long range research

BoR's Brackish Groundwater National Desalination Research Facility (BGNDRF), Alamogordo, NM

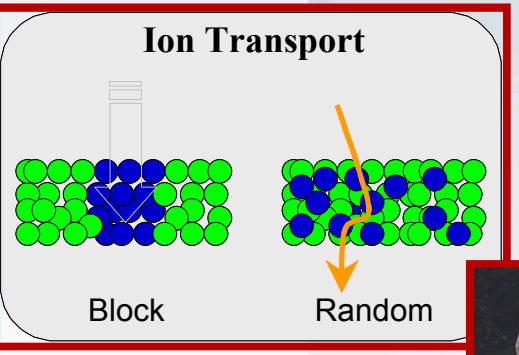
Sandia National Laboratories

Treatment Technologies: Long Range Research

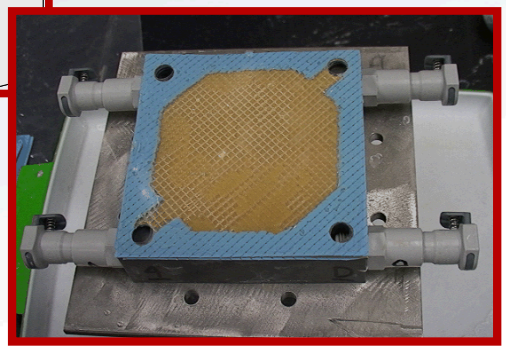


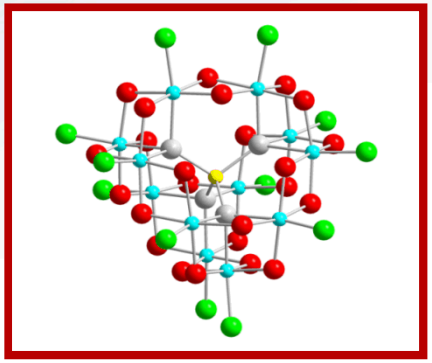
Novel Membrane Technologies

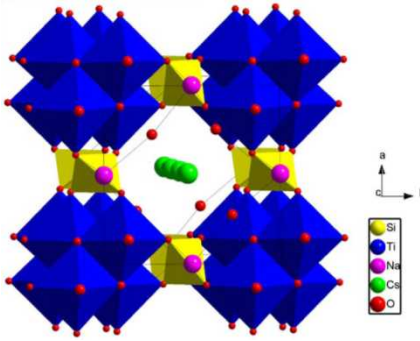
Physical and Chemical Solutions for Biofouling Control



Advanced Electrodialysis



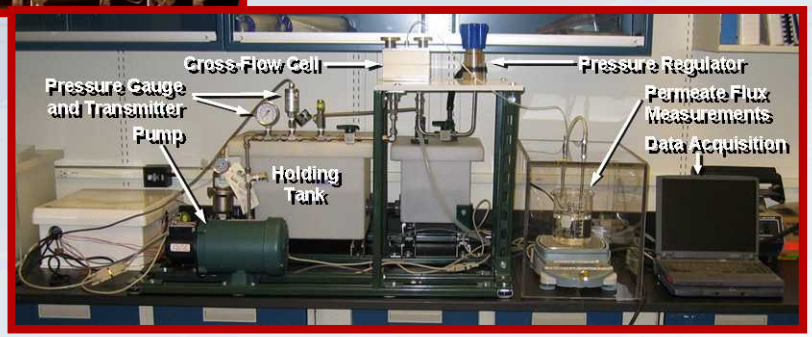




Novel Materials for Contaminant and Pathogen Removal

Sandia National Laboratories

Treatment Technologies: Jump Start Program



Sandia National Laboratories

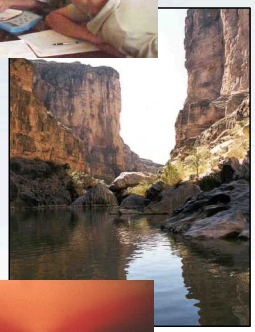
Sandia's International Water Program

Netherlands & Israel

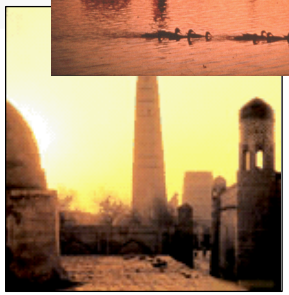
Singapore

UK

Central Asia



US/Mexico



South Asia

Jordan,Egypt & Libya

Iraq

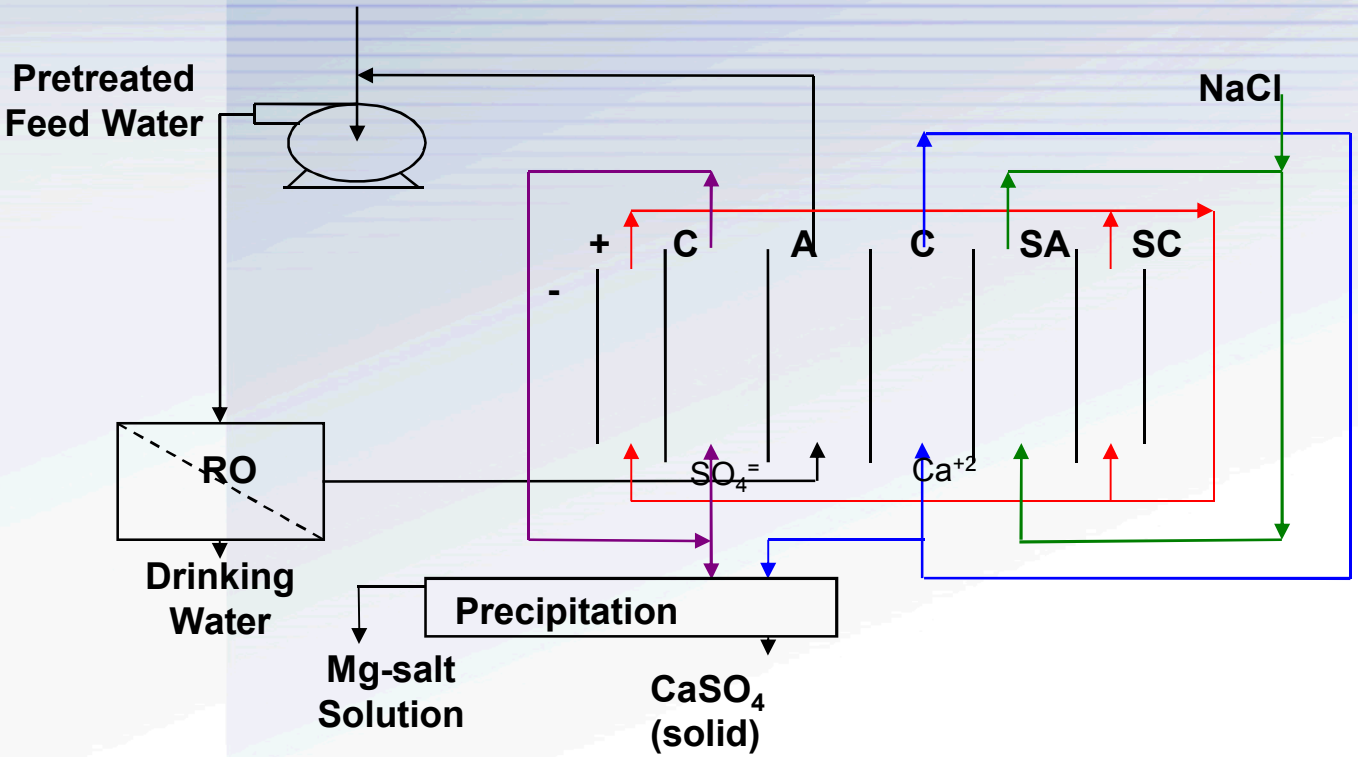
Water Program Collaborators

Backup Slides

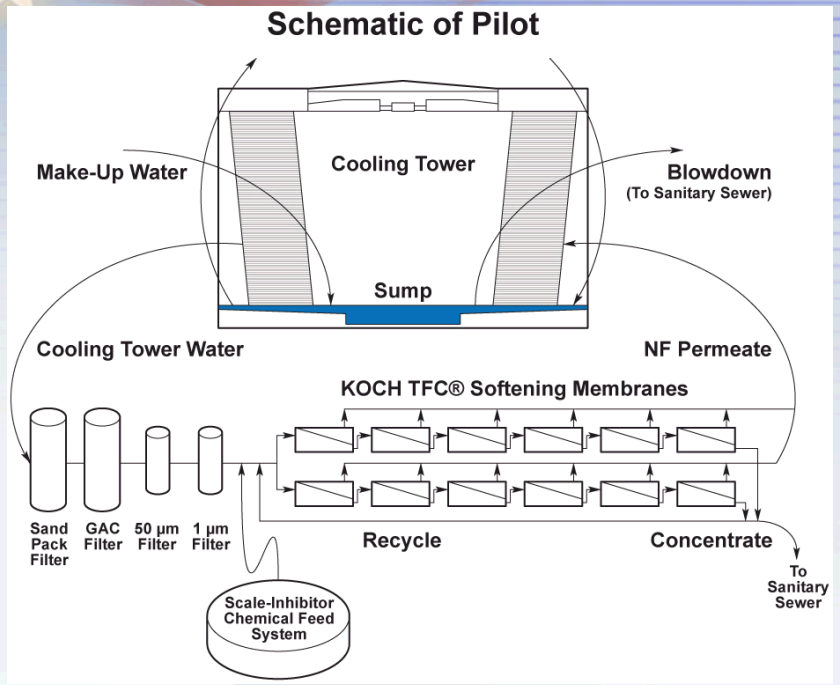
Hybrid RO/ED to Minimize Waste and Recover Saleable Products

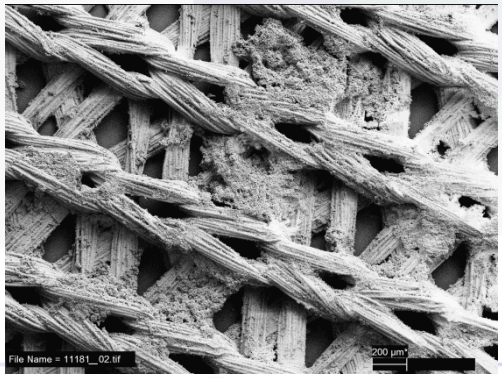
Problem: Fresh water recovery limited by low solubility of $CaSO_4$, scaling.

Technical Approach: Control scaling using a metathesis reaction scheme. Increase water recovery by removing calcium ions and sulfate ions to precipitate offline.



Nanofiltration Treatment of Side-Stream Cooling Tower Water for Reduction of Water Usage

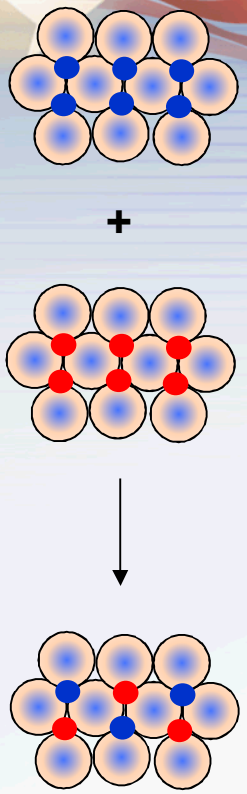




- **Water savings observed**
- **Water savings can pay for electrical costs**
- **Scaling control is critical for economic operation**

Sandia National Laboratories

Spinel Based Getters for As Removal



Trivalent Metal (Hydr)oxide ($Fe(OH)_3$, Al_2O_3)

+

Divalent Metal (Hydr)oxide ($Mg(OH)_2$, $Cu(OH)_2$, $Zn(OH)_2$)

High surface area

+

High pH_{zpc} and anion sorption capacity

<u>High surface area Spinel with high anion (e.g. arsenate, chromate) sorption capacity</u>

POC: Patrick Brady pvbrady@sandia.gov

Patent Status: Arsenic-sorbing spinel: used as filter media (U.S. Patents 7074336 B1, 7122502 B1, and 7244359 B1), coagulant and lime softening aid (U.S. Patents 7138063 B1 and 6802980 B1), and can be formed *in situ* to decontaminate soils/aquifers (U.S. Patent 683695 B1).

In Tank Recirculation Treatment System

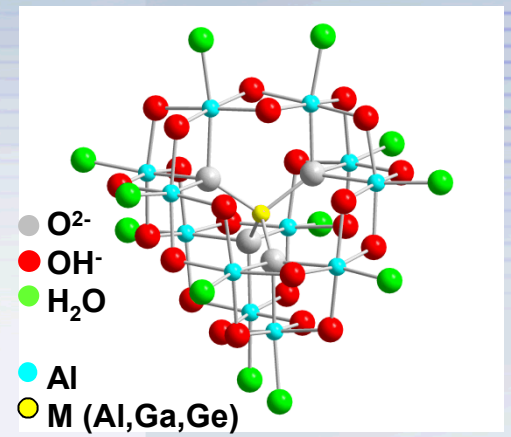
Designed to reduce the levels of a variety of organic and inorganic contaminants in water storage tanks.

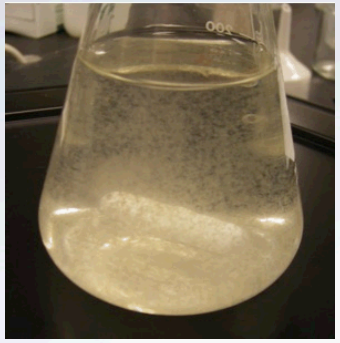
POC: Brian Dwyer bpdwyer@sandia.gov

Patent Status: US Patent #7514004 In-Tank Recirculating Arsenic Treatment System

Strategies for Controlling SiO_2 Scaling

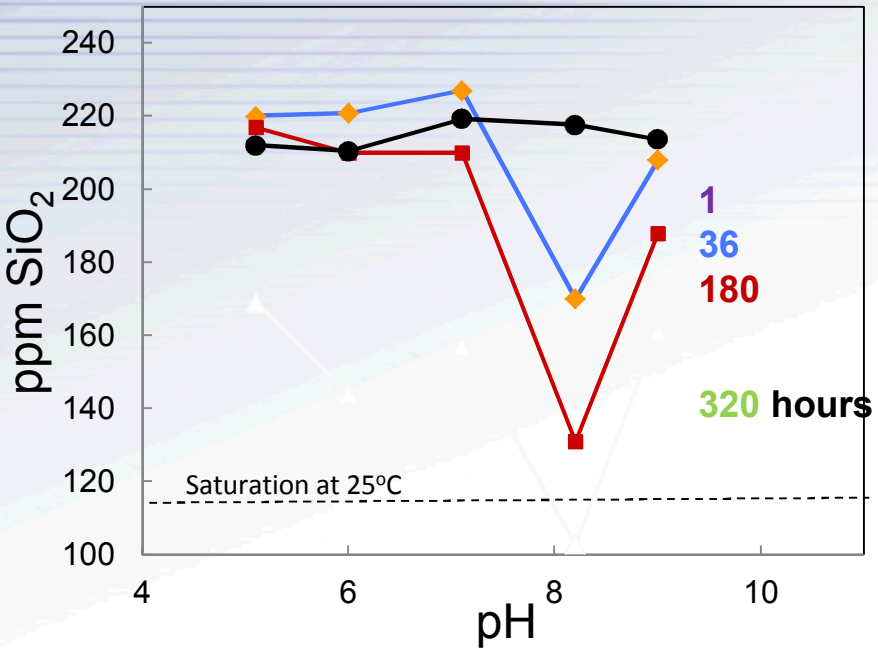
Coagulation of SiO_2





Simple aluminum-based agents are effective, simple, and compatible with other industrial processes.

pH Control to Delay of SiO_2 Precipitation

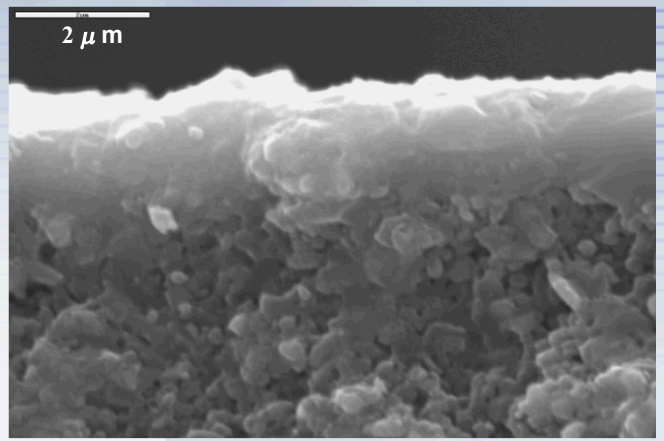


Lowering solution pH decreases equilibrium calcite solubility and kinetic rates of silica polymerization.

Sandia National Laboratories

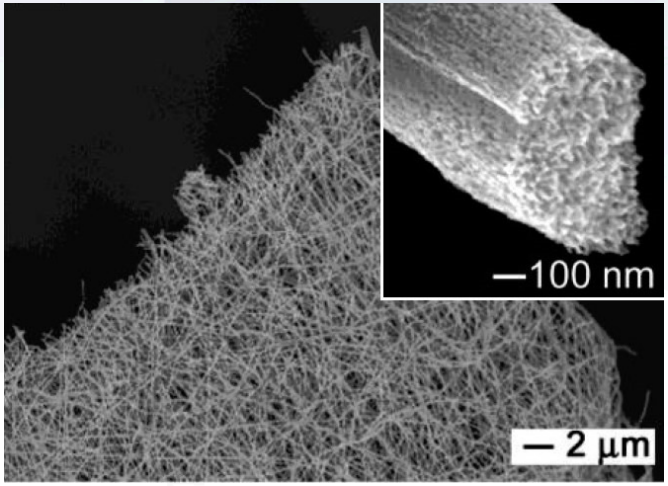
Future Research Challenges and Opportunities: Science & Technology Efforts for Advanced Filtration

- **Nanoporous Zeolite and Metal Organic Framework (MOF) Materials**



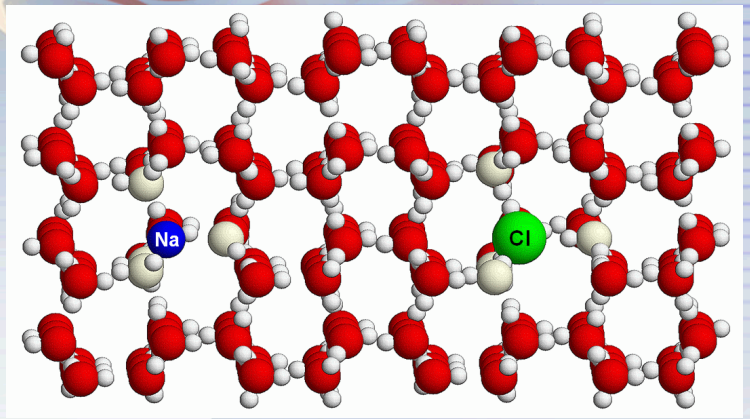
MFI zeolite membrane (0.74 nm nanopore dimension) – cross-sectional, on porous alpha-alumina. Past interfacial water research (coupled with modeling) has identified the role of water in molecular sieve pores with respect to cation selectivity.

- **Nanoporous Electrospun Nanofibers**

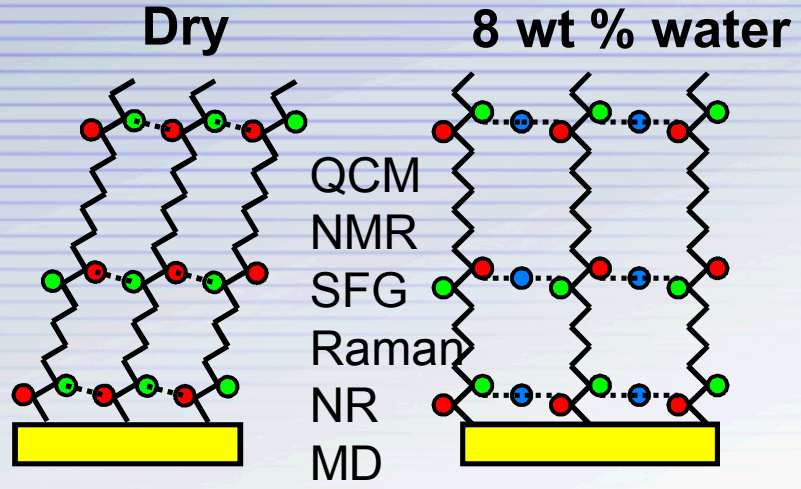


An electrospun nanofiber (inset) showing nanoporosity. A mat of these materials (larger figure) can be tuned with tuned microporosity, coupled with nanoporosity within the nanofiber. The use of functionalization (by various potential approaches) can further tune filtration properties.

Exploiting Interfacial Water Properties for Desalination and Purification Applications



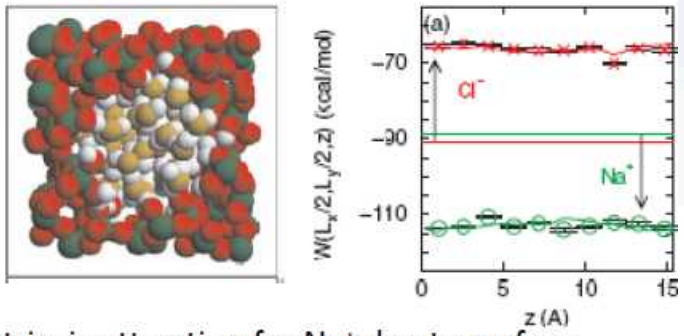
Density Functional Theory Models of Na-Cl Solvation in Ice



Crystalline, rigid Amorphous, fluxional

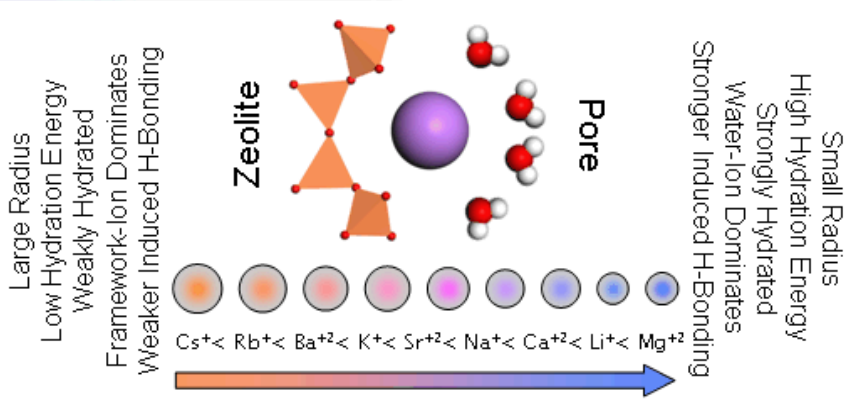
Water Restructures Polymer Films

Combined DFT, AIMD, and force field studies of electrolyte permeation in nanopores



intrinsic attraction for Na^+ due to surface dipoles in hydroxylated silica nanopores

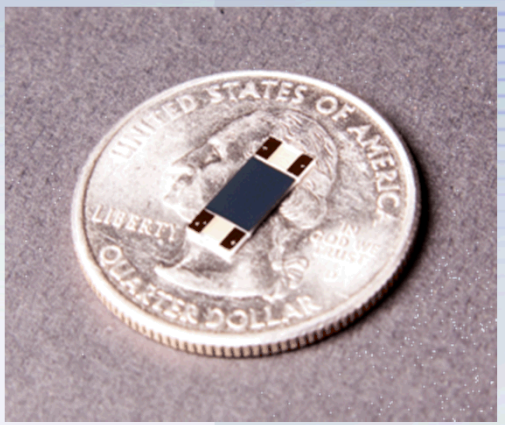
Leung, Rempe, & Lorenz, PRL 96:095504 (2006)



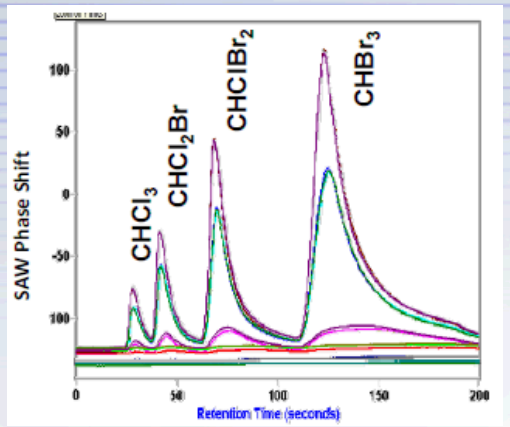
Sandia National Laboratories

Future Research Challenges and Opportunities: Science & Technology Efforts for (Inexpensive) Detection

Nanoporous Carbon (NPC) Coated SAW Device System for sub PPB Detection of Trihalomethanes in Water

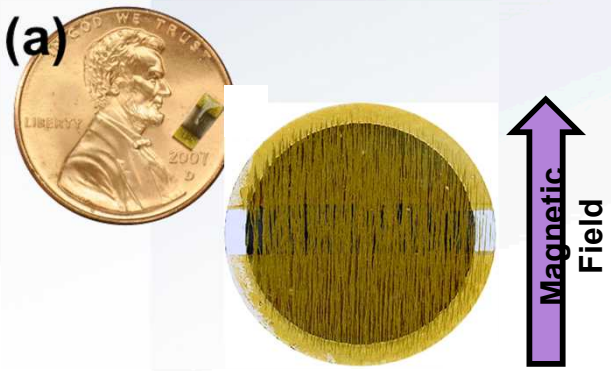


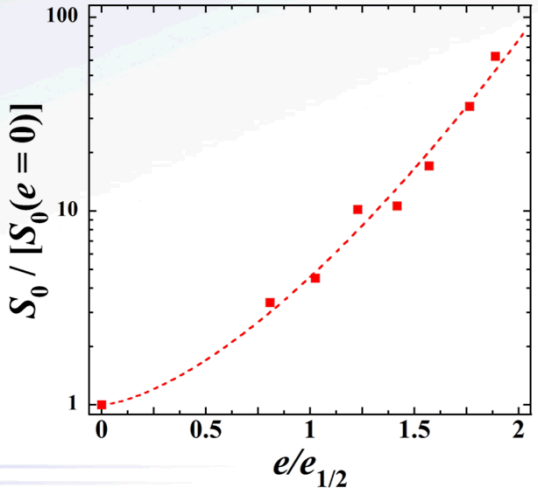
NPC coated SAW (Surface Acoustic Wave) detector



Detect and speciate > 17 different chemicals in water.

Field-Structured Chemiresistors: Tunable Sensors for Chemical-Switch Arrays





Response tunability enables analyte concentration to be measured over a 4-decade range. Response time is concentration independent and analyte dependent.

Sandia National Laboratories