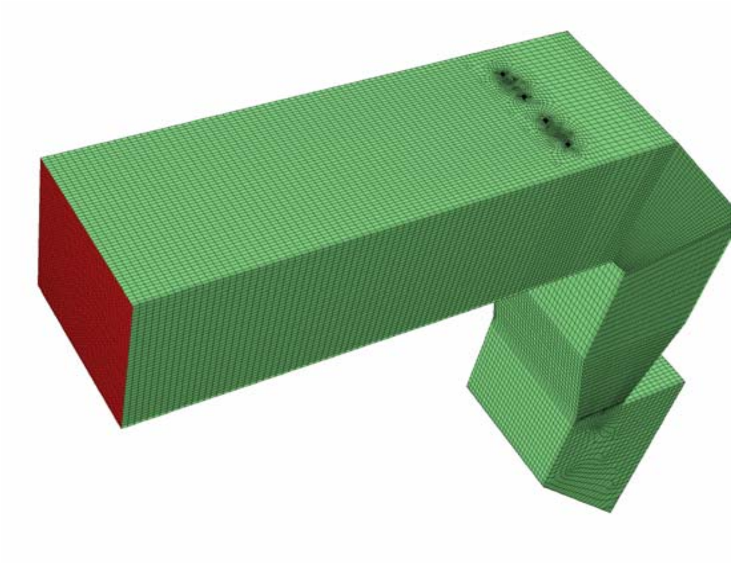
Computational Approaches to the Development of Advanced Mercury Control Technologies



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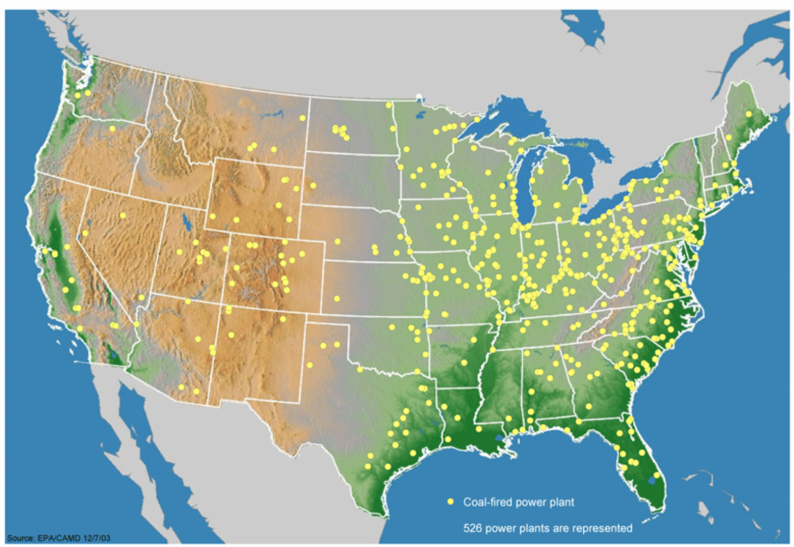
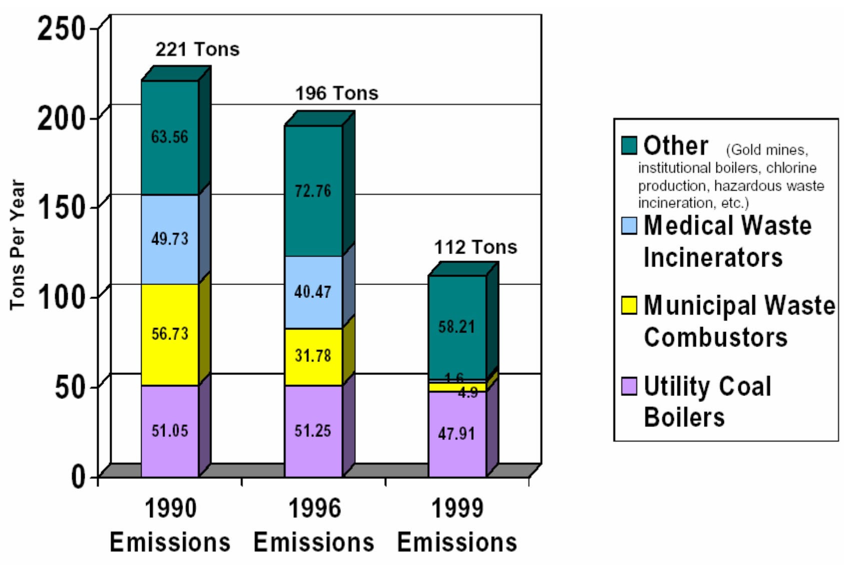
DOE/NETL's Mercury Control Technology R&D Program Review, **Pittsburgh, July 12-14, 2005**

Goals and Objectives
Programmatic Drivers

- **Mercury is the hazardous air pollutant of greatest public health concern***
- **There are about 1,100 coal-fired units in the US**
  - **These contribute more than 40% of man-made mercury emissions (~50 tons/year)**
  - **Other sources have been reduced, but utility emissions remain unchanged**
  - **Clean Air Mercury Rule will regulate emissions using cap-and-trade approach**



U.S. Coal-Fired Power Plants



* EPA Study of Hazardous Air Pollutant Emissions from Electric Utility Steam Generating Units – Final Report to Congress (1998)

Goals and Objectives
Programmatic Goals

- DOE/NETL Mercury Control Technology Field Testing Program
  - Prepare technologies for commercial demonstration by 2007
  - Reduce "uncontrolled" Hg emissions by 50-70%
  - Reduce cost by 25-50% compared to baseline cost estimates
    - Baseline Costs: $50,000 - $70,000 / lb Hg Removed

- More than 70% of US coal-fired boilers use ESPs for particulate control
  - Activated Carbon Injection (ACI) is a feasible technology for these units
  - Need to understand the mechanics of in-flight capture

- ACI field testing activities
  - Absolutely essential in terms of advancing this technology
  - Approach problems with a hammer
    - Limited knowledge of the mass-transfer processes in duct (sorbent- to duct-scale)
    - It is not always possible to interpret test data based on current understanding

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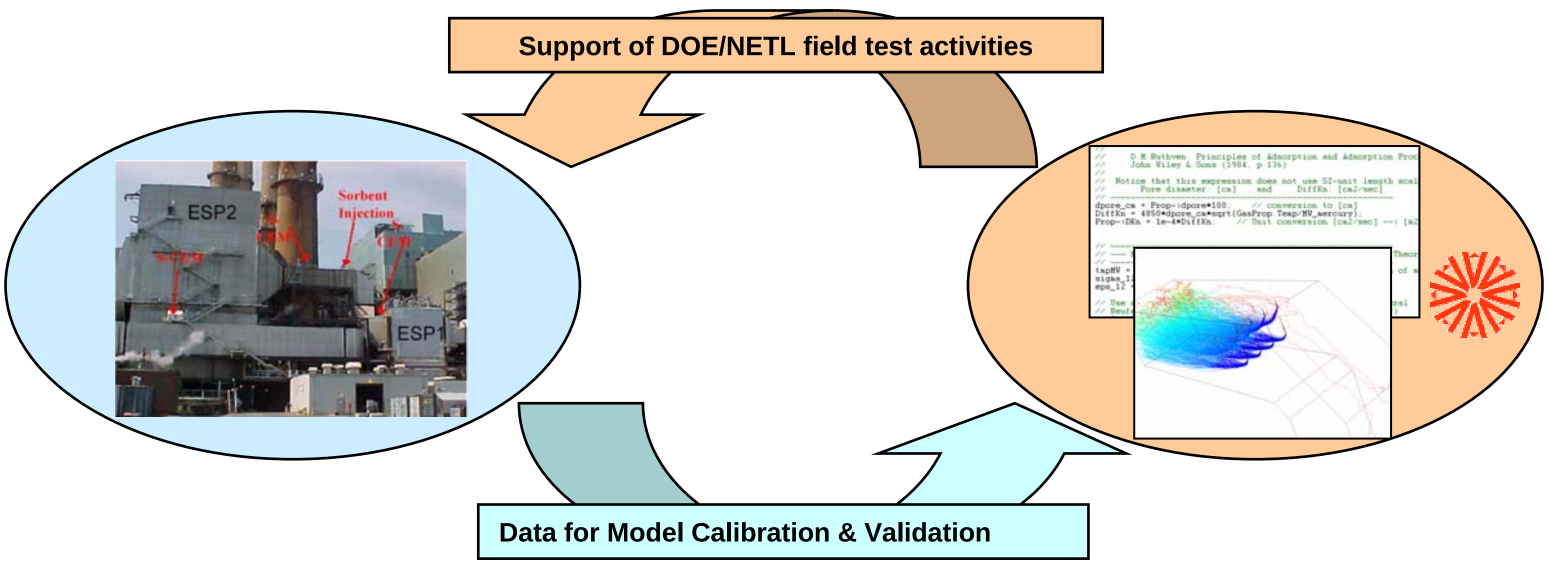
Goals and Objectives

Potential Benefits of Computational Flow Modeling

<u>Use CFD-based tools to simulate and improve the understanding of sorbent-based mercury control processes</u>

- Detailed information provided
  - Flue gas flow (local conditions)
  - Sorbent dispersion and residence time
  - Where the capture takes place
- Practical questions answered
  - Optimize injection grids
  - Predict necessary sorbent feed rates
  - Enables inexpensive and quick what-if studies

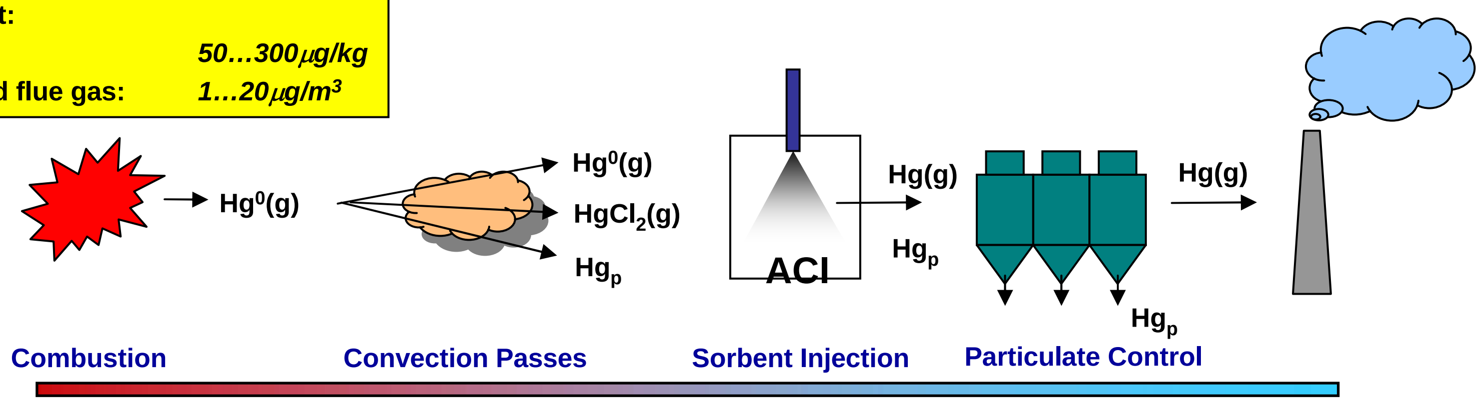


Technical challenges

Mercury speciation

- **Mercury only present in trace amounts (ppb-range)**
  - **Simulation of mercury capture as a post-processing step**
- **Mercury speciation in coal-derived flue gases**
  - **Important as it influences mercury capture efficiency**
  - **Speciation chemistry is kinetically controlled**
    - **Between 35 and 95% of mercury is oxidized**
    - **Speciation remains fixed at typical sorbent injection temperatures (120-200ºC)**
- **Computational models must factor in partitioning between Hg(o) and $HgCl_2$**
  - **Transport and adsorption of these two compounds is computed separately**
  - **Identical transport mechanisms. Differences in species diffusivity and adsorption rates**
  - **Initially assuming frozen speciation chemistry (known oxidation fraction)**

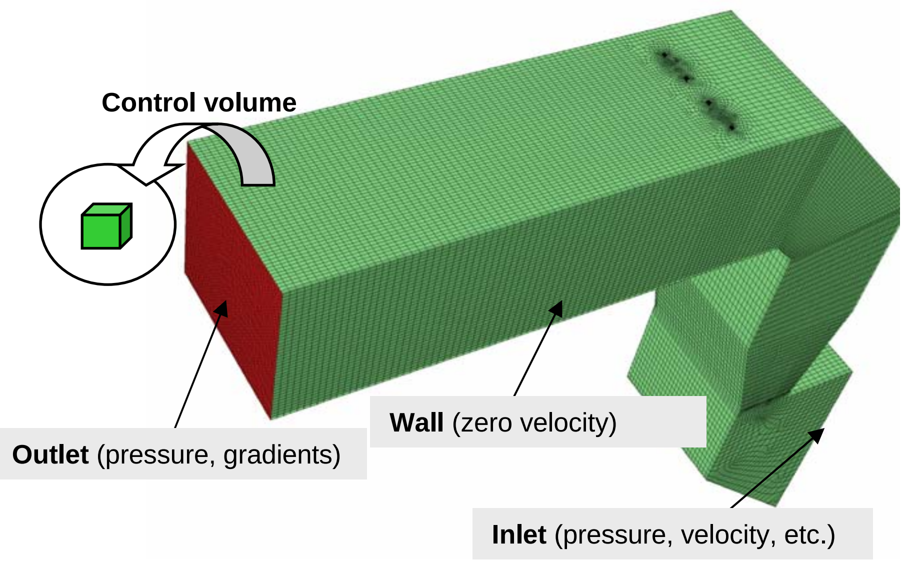
Mercury content:	
in coal:	*50…300μg/kg*
in coal-derived flue gas:	*1…20μg/m³*



Technical Approach

A Brief Introduction to Computational Fluid Dynamics (CFD)

- **CFD process entails**
  1. **Discretization of fluid region into a finite set of control volumes (mesh)**
  2. **Solution of general transport equations**
     - **Conservation of mass, momentum, energy, species, etc.**
  3. **Conservation obtained via integration of transport equations over control volumes**
  4. **Application of proper boundary conditions**



$$\underbrace{\frac{\partial}{\partial t}\int_V \rho\varphi \, dV}_{\text{Unsteady}} + \underbrace{\oint_A \rho\varphi V \cdot dA}_{\text{Convection}} = \underbrace{\oint_A \Gamma \nabla\varphi \cdot dA}_{\text{Diffusion}} + \underbrace{\int_V S_\varphi \, dV}_{\text{Generation}}$$

Equation	φ
continuity	1
x-mom.	u
y-mom.	v
z-mom.	w
energy	h

Technical Approach

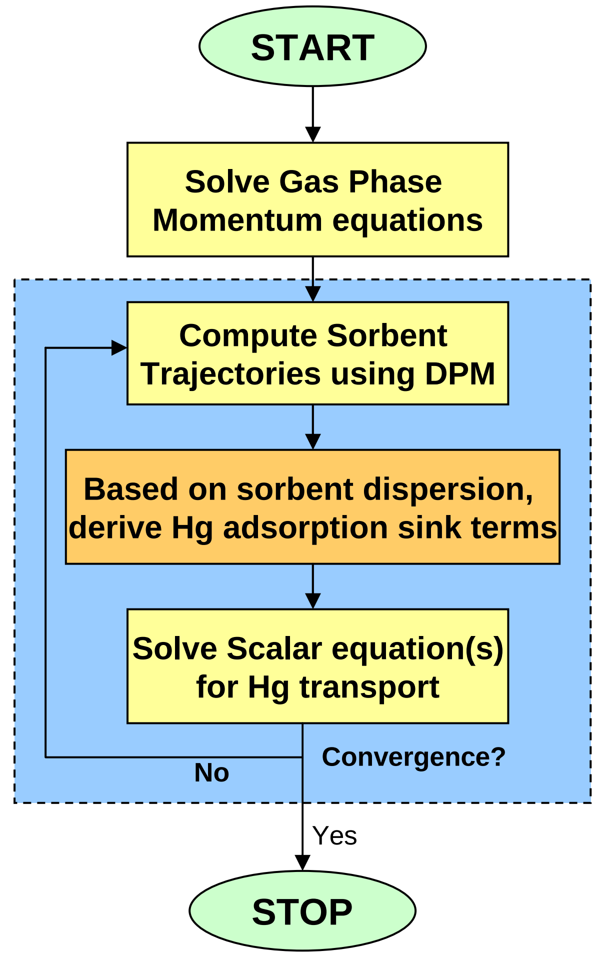
Mercury Capture Modeling

- **Mercury transport equation(s) solved in ductwork**
  - **Determines distribution of gas-phase mercury in duct**

$$\frac{\partial}{\partial x_i}\left[\rho u_i c_g - \frac{\mu_t}{Sc_t}\frac{\partial c_g}{\partial x_i}\right] = S_{Hg}$$

sink term

- **Lagrangian tracking of sorbent particles**
  - **Mercury sink terms updated during tracking**
  - **Particle sub-model**
    - Internal mercury concentration profiles $C_p(r)$
    - Sorbent utilization $(\omega/\omega_{max})(r)$
- **Iterative procedure (tracking / Hg transport)**
  - **Intraparticular transport and adsorption driven by concentration gradients**



Technical Approach

Mass Transport and Adsorption inside Sorbent Particle

- **Mercury adsorption takes place in three steps:**

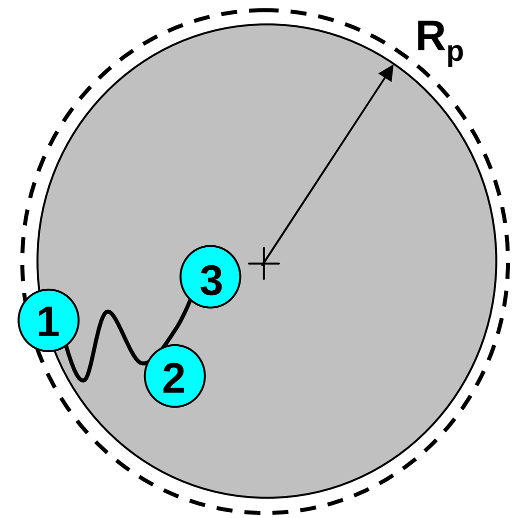
1. **Mass transfer from gas phase to external sorbent surface (film resistance)**

2. **Diffusion mass transfer through porous structure**
  - **Knudsen Diffusion (function of pore diameter ao.)**

3. **Surface adsorption on internal surfaces**
  - **Adsorption equilibrium given by Langmuir isotherm**
  - **Appears as sink term in the particle sub-model**

$$\Re = k_1 \omega_{max} \underbrace{\left[1 - \frac{\omega}{\omega_{max}}\right]}_{\text{Unused fraction}} c_p - k_2 \omega$$

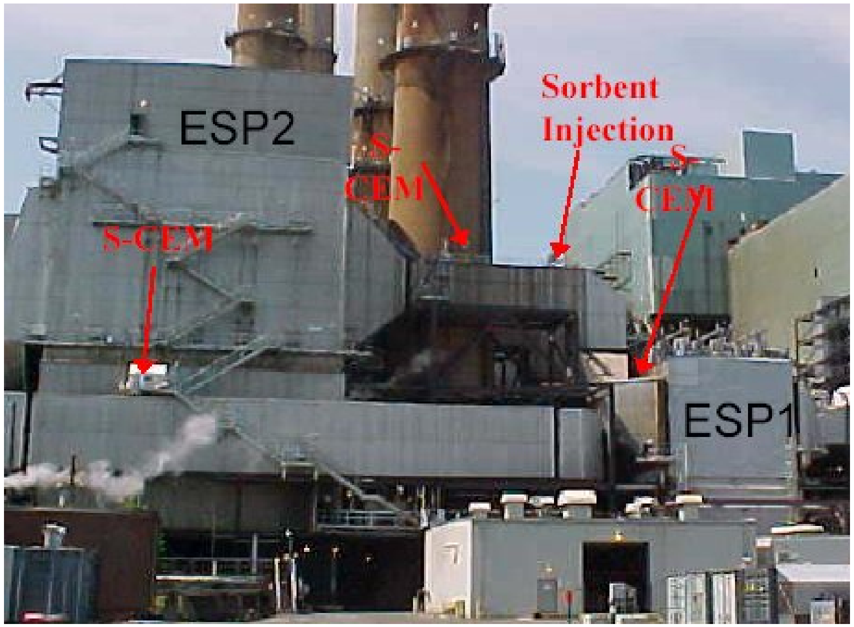
Idealized sorbent particle (perfect sphere)

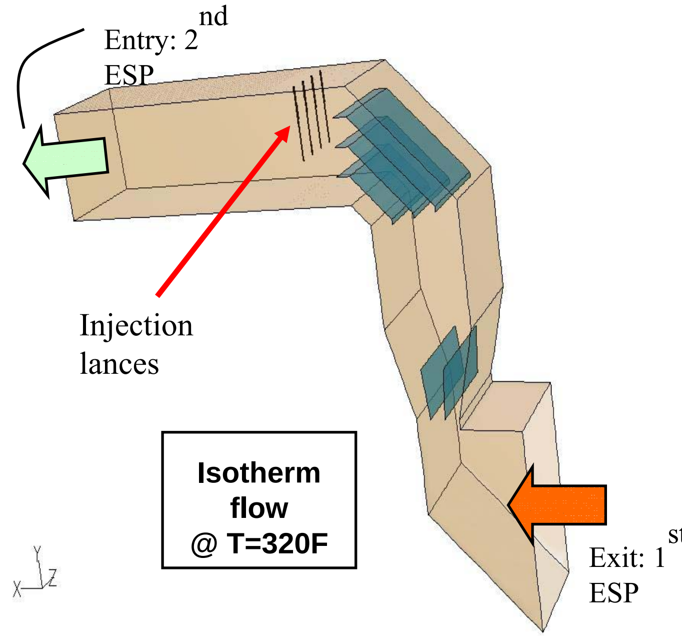


Pulverized activated carbon
Porous structure (pore radius 5-100 Å)
Large internal surface area (600–1,200 m2/g)

Application Examples

Brayton Point Power Plant – Phase I field test site

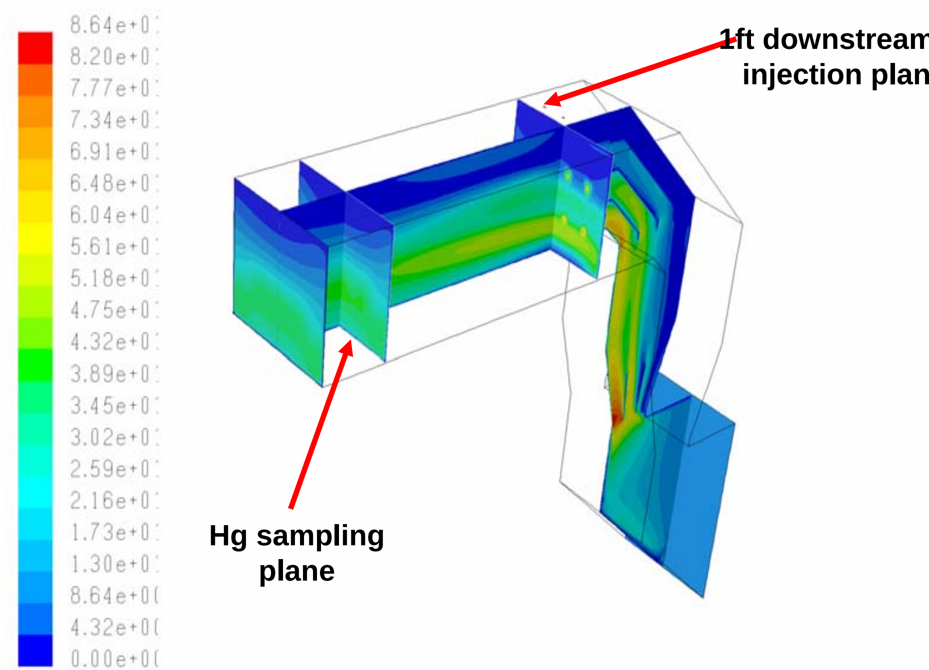




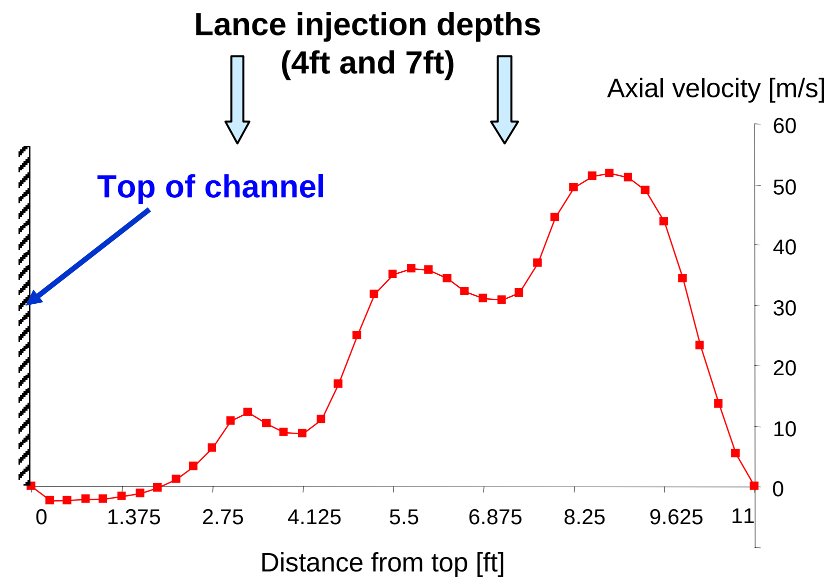
- **ACI tests 2002 as part of the DOE/NETL Mercury Control field test program**
- **Power plant equipped with two electrostatic precipitators**
  - **Injection of activated carbon via set of eight lances upstream of the 2nd ESP**
  - **Lances are introduced in pairs via four ports**

Application Examples

Brayton Point Power Plant – Gas phase flow



Velocity magnitude plot

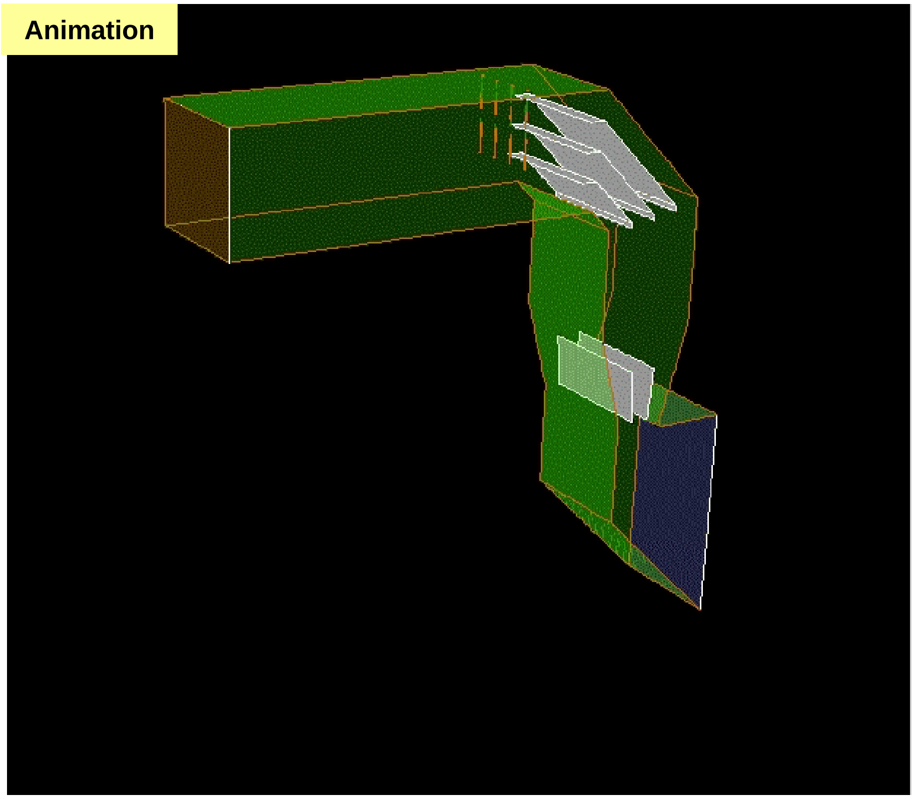


Velocity profile recorded in 2nd port

- **Flue gas flow inside injection duct is very non-uniform**
  - **Flow predominantly travels in lower half of duct**
  - **Stair-cased velocity profile is an effect of (three) upstream turning vanes**
  - **Injection lances are long enough to penetrate separation zone**

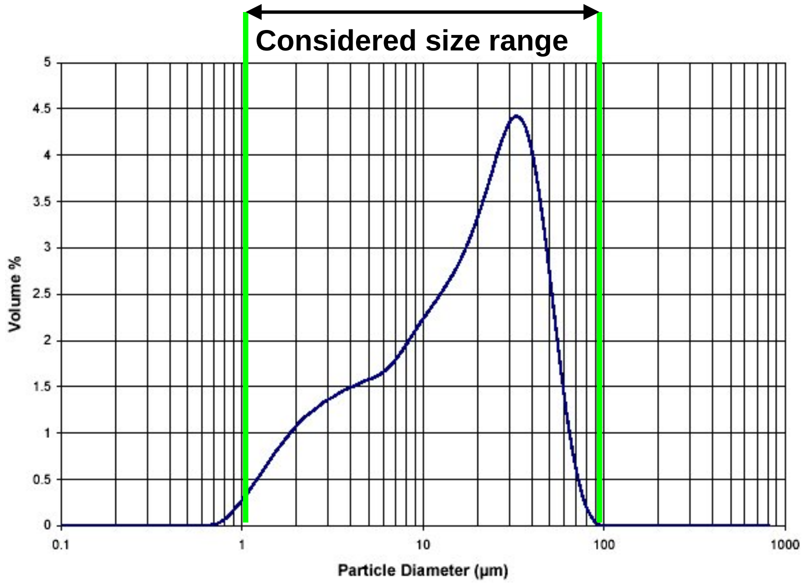
Application Examples

Brayton Point Power Plant – Sorbent trajectories



Trajectories of injected sorbent

Colored by residence time



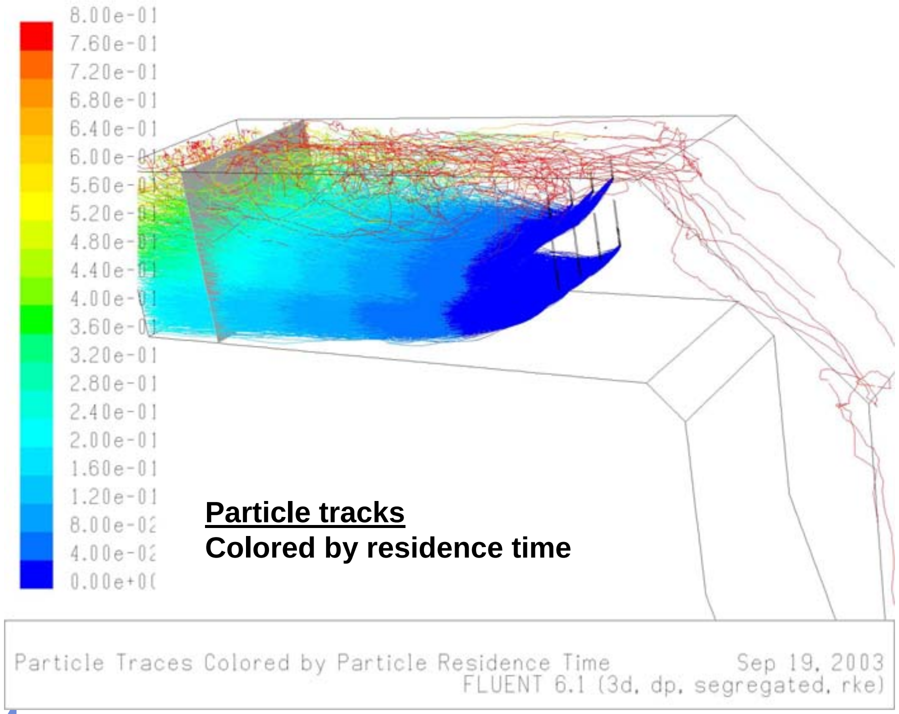
Darco FGD
Particle Size Distribution (PSD)

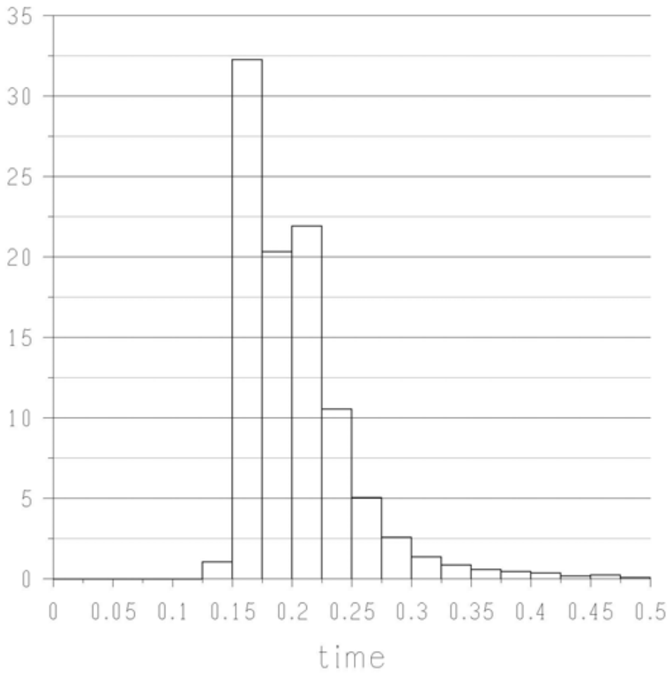
- **Ten size bins (d_p= 1 …100µm)**
- **Trajectory flow rates weighted based on PSD**

Application Examples

Brayton Point Power Plant – Sorbent residence time

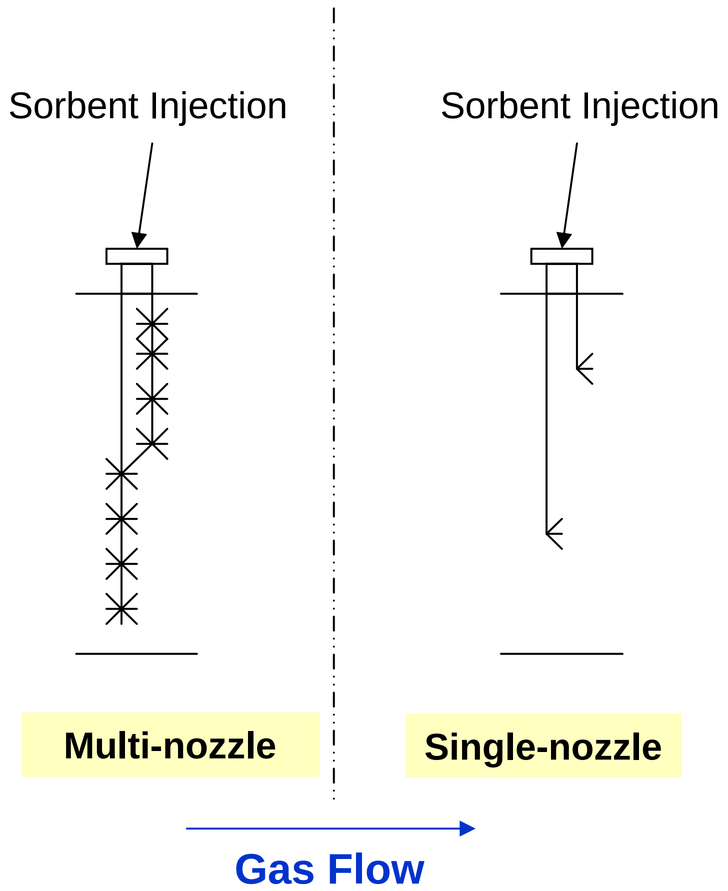
- **Short injection duct → residence time has been a concern**
  - **From simple plug-flow assumption, t_{res} can be estimated as ~0.45sec.**
  - **Most sorbent travels where gas velocities are above average**
  - **Actual sorbent residence time is lower than estimated (approx. 0.2sec)**





Application Examples

Simulation of Flow in Multi-Nozzle Injection Lance

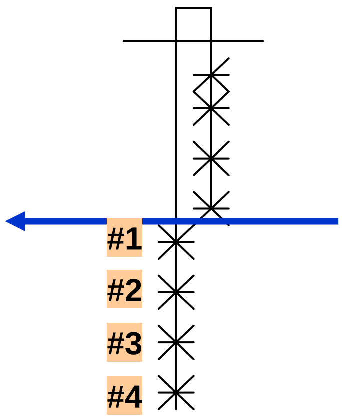


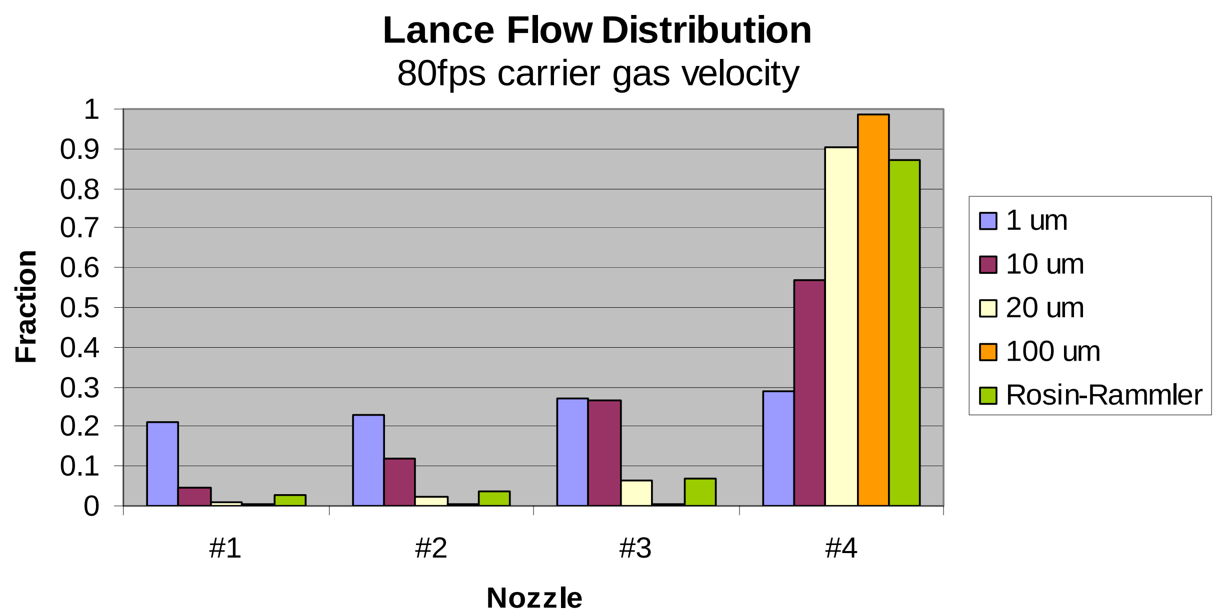
- Two lance designs tested at Brayton Pt.
  - Insignificant difference in capture
- Multi-nozzle lance design
  - Determine sorbent split between nozzles
  - Information used for proper specification of injection flow rates in overall duct model

Application Examples

Multi-Nozzle Injection Lance – What is the sorbent split?

Multi-nozzle
injection lances

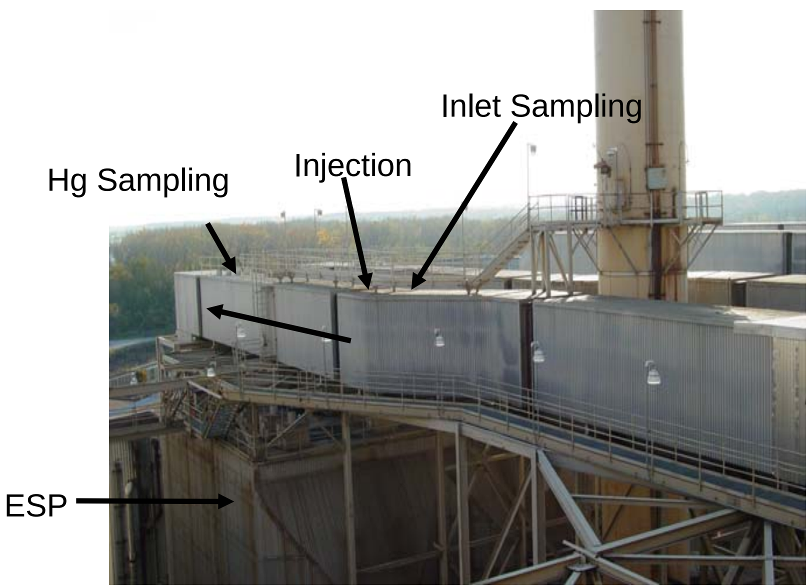


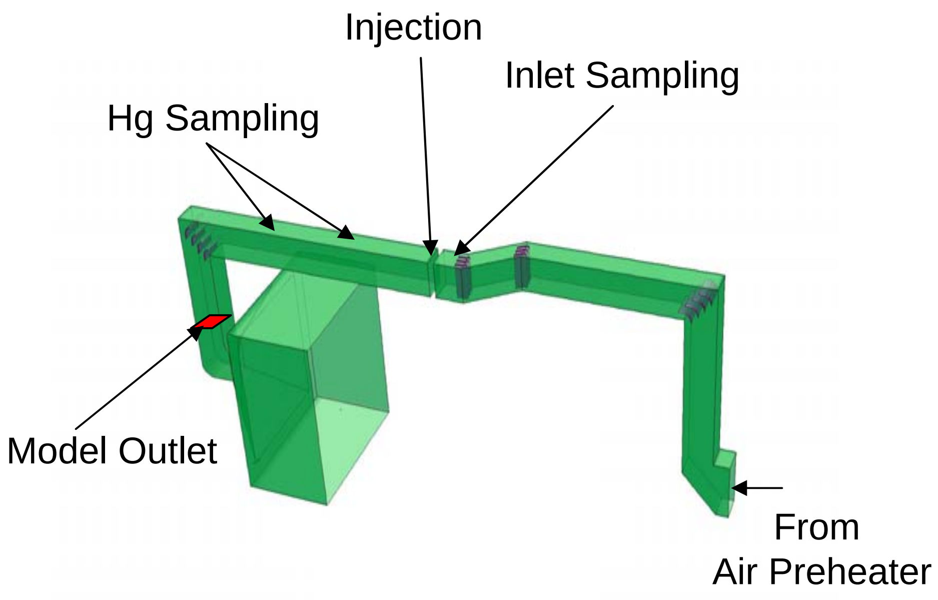


- **Gas Flow is almost evenly split between eight nozzles of lance**
- **How is the injected sorbent distributed between individual nozzles?**
  - **Most sorbent exits lower nozzles (~85-90%)**
  - **Performance very similar to that of a much simpler single-nozzle lance**
  - **May explain findings at Brayton Point (capture insensitivity to lance design)**

Application Examples

AmerenUE Meramec – Phase II field test site

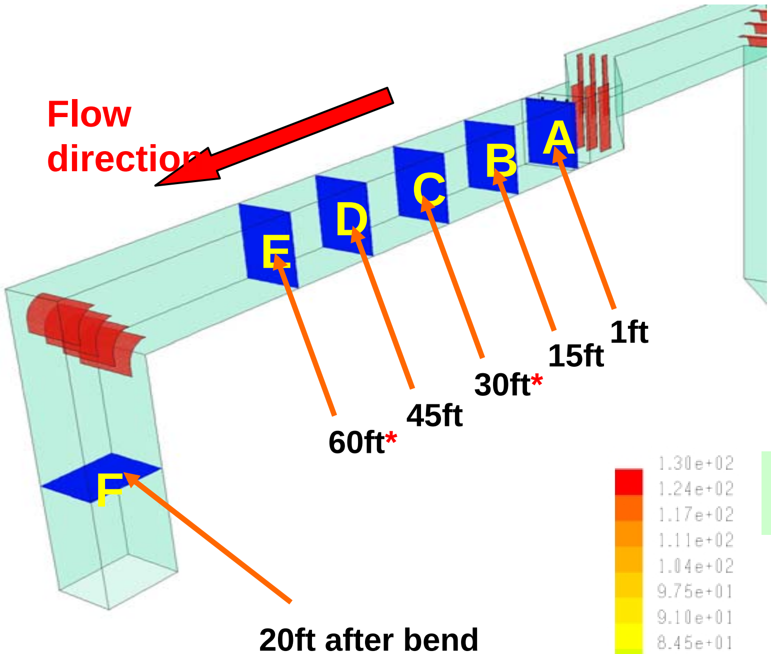




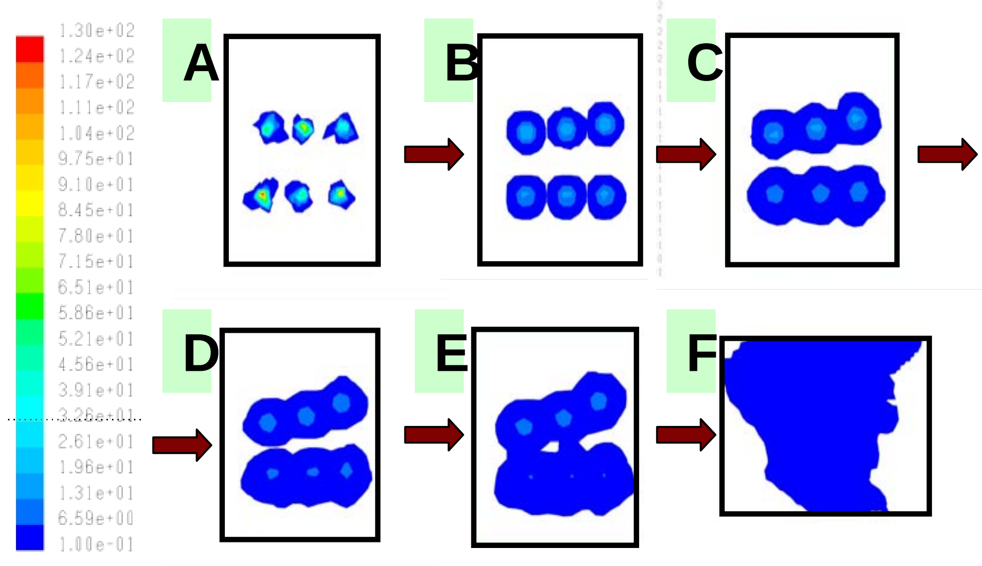
- **ADA-ES completed testing in 4th quarter 2004**
  - **Carbon Injection via six single-nozzle lances inserted through three ports**
  - **More than 100ft of duct provides long residence time for capture**

Application Examples

Meramec – Dispersion patterns



Coverage with >10% of average sorbent conc.



* Mercury sampling planes

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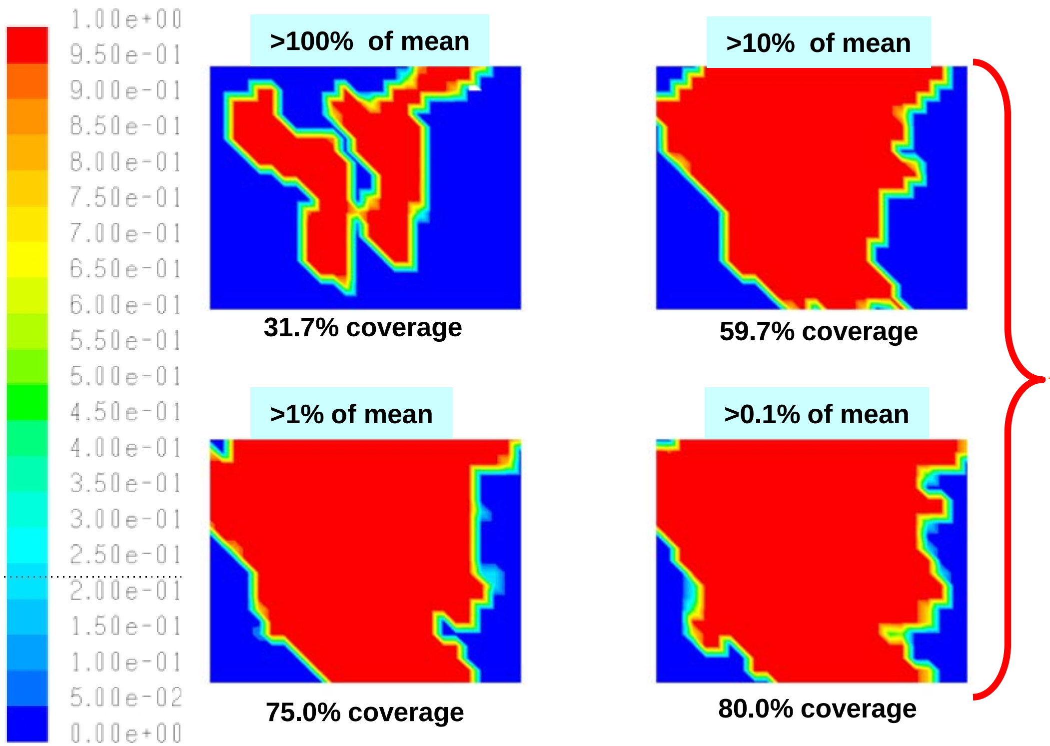
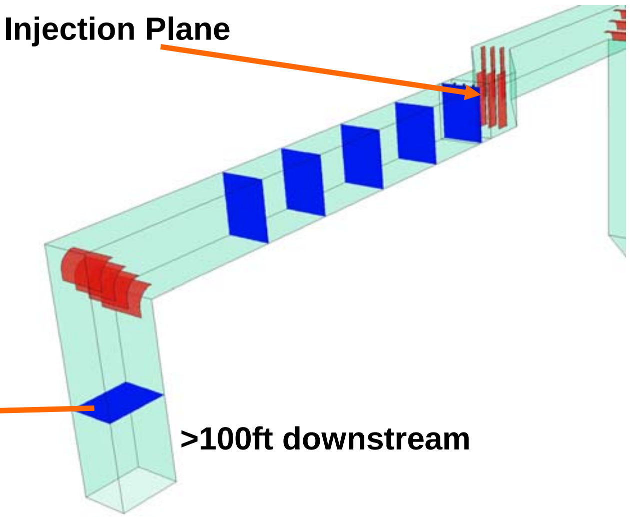
Application Examples

What sorbent concentration is sufficient for capture?

No-one knows!

Plane F – Coverage at different cut-off ratios





Law of Diminishing Returns

Filter function (step-function)

Low concentrations $c_{sorb} < c^*$ → $c_{sorb,filtered} = 0.0$

High concentrations $c_{sorb} > c^*$ → $c_{sorb,filtered} = 1.0$

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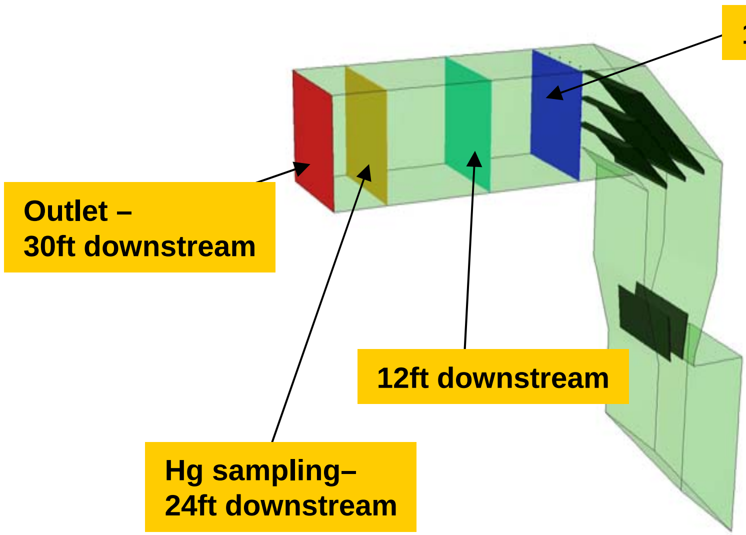
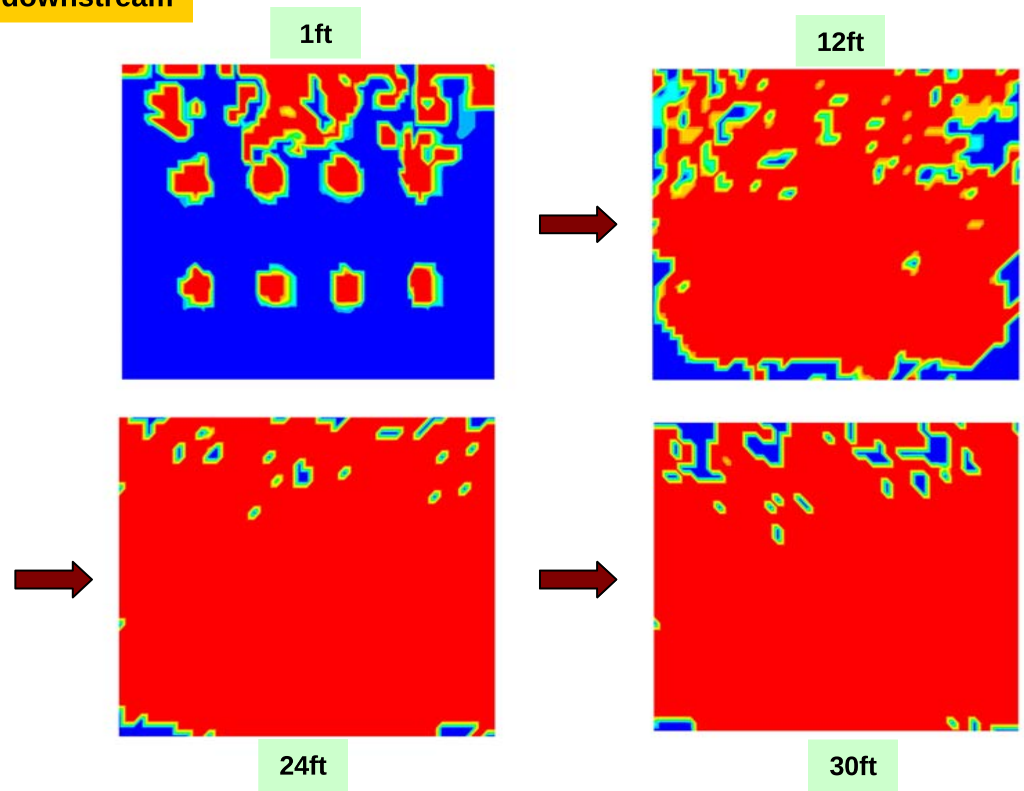
Application Examples

Comparison between Brayton Point and Meramec





Coverage with >10% of average sorbent conc.

Application Examples

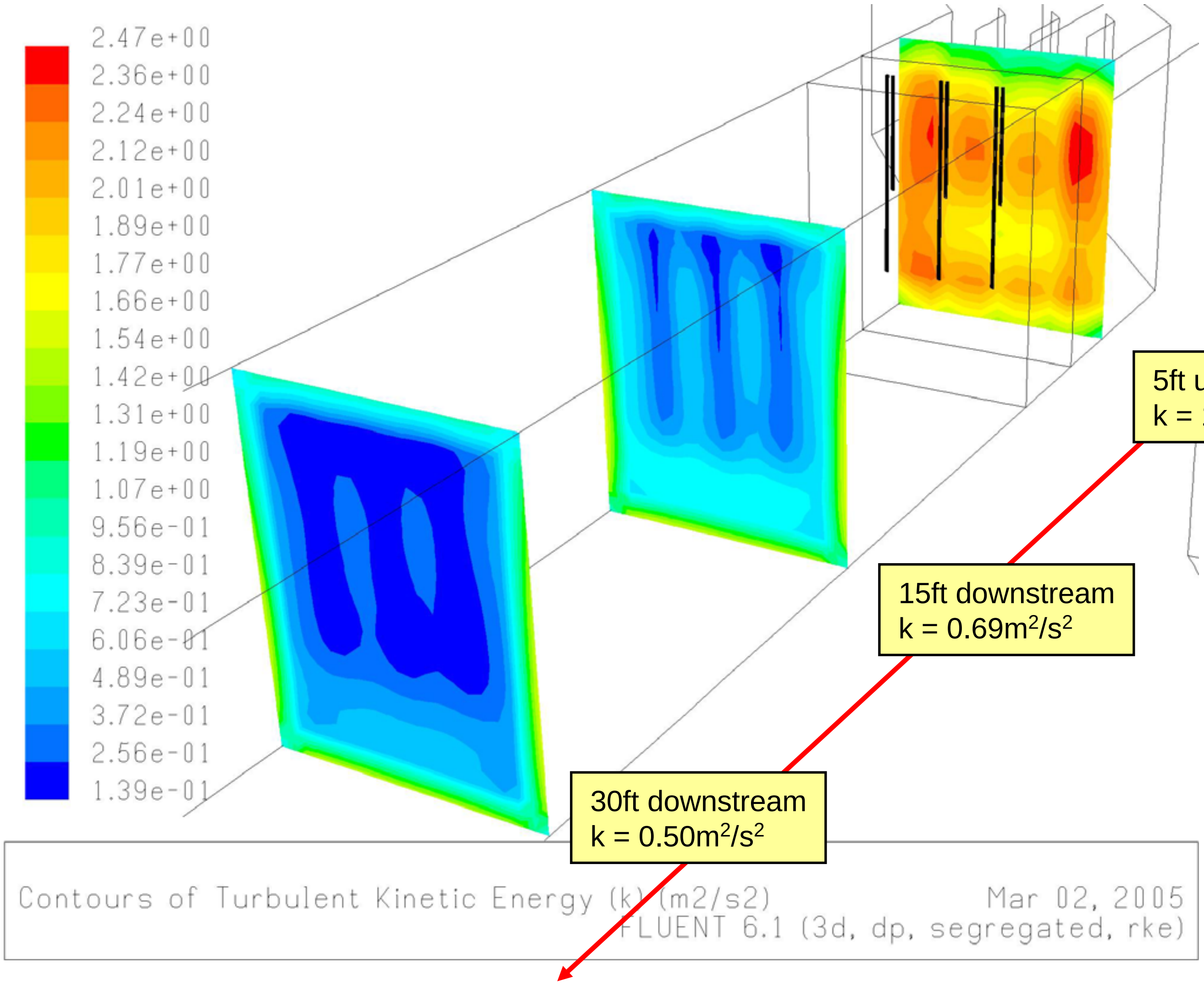
Comparison between Brayton Point and Meramec

- **Dispersion** is **remarkably better** at Brayton Point than at Meramec
  - Identical sorbent (Darco FGD)
  - Similar duct dimensions (11 x 12ft versus 10¼ x 8ft2in)
  - Mean gas velocity is a little higher at Brayton Pt. (~70fps versus ~50fps)
- Enhanced dispersion is caused by **turbulent mixing**

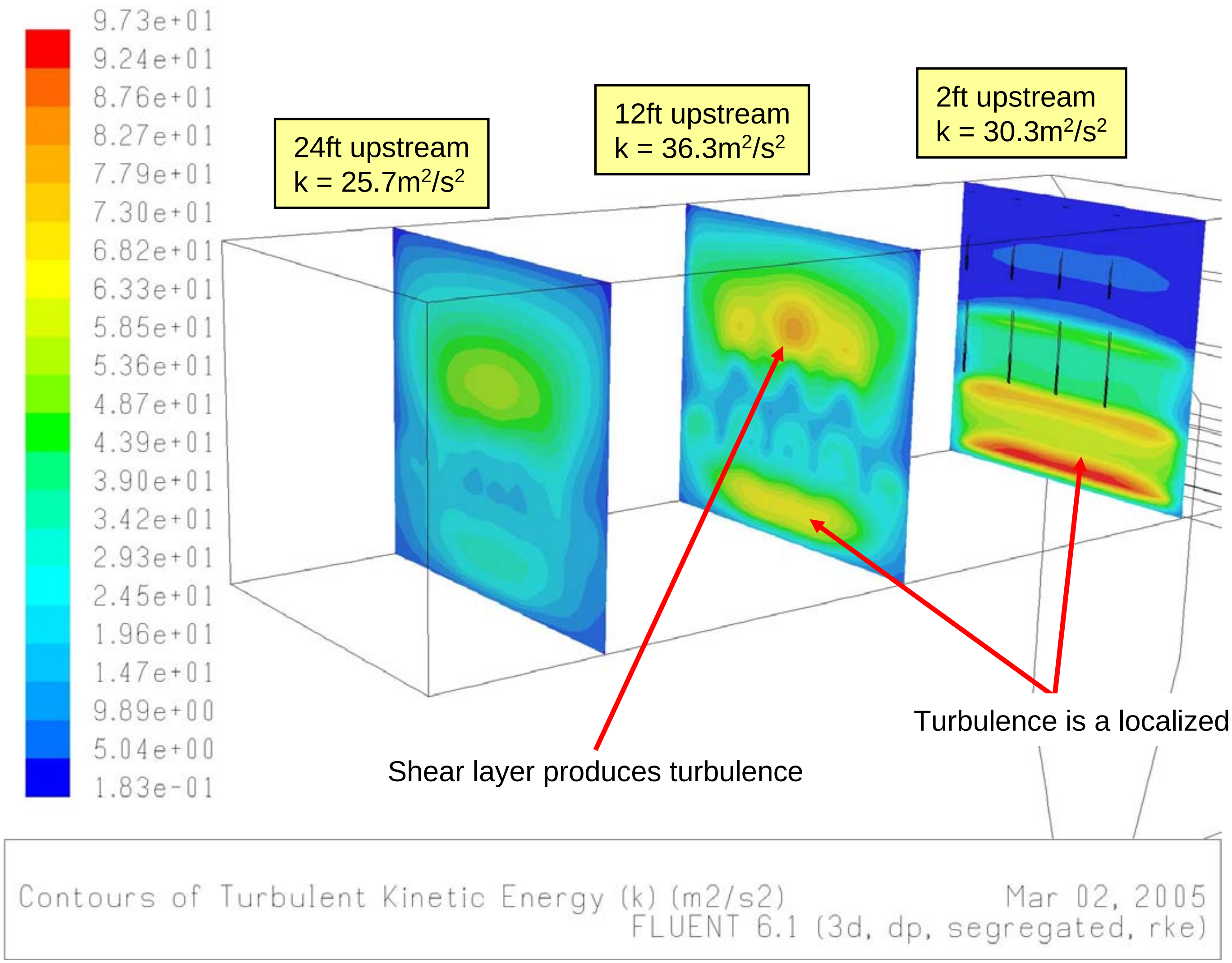
Downstream Distance from Injection	*Brayton Point* Coverage Fraction		*Meramec* Coverage Fraction		Downstream Distance from Injection
	>100% avg.	>10% avg.	>100% avg.	>10% avg.	
1ft	0.069	0.221	0.049	0.056	1ft
12ft	0.224	0.840	0.125	0.187	15ft
24ft	0.282	0.970	X	X	No comparable sampling plane
30ft	0.307	0.944	0.164	0.296	30ft

Application Examples

Meramec Turbulent Kinetic Energy

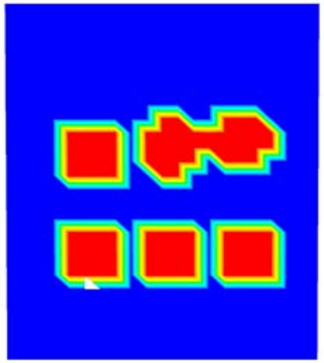


Application Examples
Brayton Point Turbulent Kinetic Energy



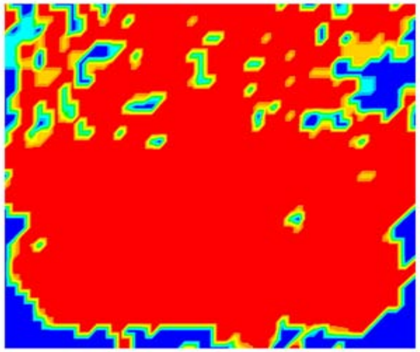
Application Examples
Comparison between Brayton Point and Meramec

MERAMEC



15ft after injection

BRAYTON PT.



12ft after injection

- **Enhanced dispersion is caused by turbulent mixing**
  - **Turbulent energy an order of magnitude higher in the Brayton Pt. injection duct**
  - **Can turbulence be induced to enhance mixing?**
    - **Interesting approach for tight retrofits with short residence time**
- **Notice that in spite of sub-par dispersion, mercury capture at Meramec was quite good**
  - **Higher residence time**
  - **Higher mercury level in flue gas**

Work Scope FY06

Main Focus FY06:

- **Continue support of DOE/NETL ACI field testing**
  - **Currently putting together models for two Phase II test sites: Monroe and Yates**
  - **Identify further sites for modeling once Phase III projects have been awarded**

- **Continue Capture Model Development**
  - **Finish model implementation with frozen chemistry**
    - Revisit past field test site models for validation
  - **Extend CFD-based mercury capture modeling capabilities to include chemical kinetics that describe the speciation of mercury**
    - Will enable prediction of capture efficiency trends such as the impact of flue gas chlorine conc.
    - May eventually expand scope to include CFD modeling of mercury capture in scrubber systems

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Thanks!