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# *Modeling of Entrained Flow Mercury Adsorption on Sorbents*

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# Background

- A 1997 EPA report to Congress cited mercury as a pollutant of immense danger to humans.
- Coal-fired power plants are the largest single source of anthropogenic mercury in the United States.
- New methods to capture mercury are being developed to prevent Hg escape into the atmosphere.



# Objective

- Develop an experimental system to investigate the contributions of entrained flow mercury capture via sorbents
- Develop a model to predict the adsorption of Hg from entrained flow systems
  - Include intra-particle effects
  - This presentation focuses on effects of internal and external particle mass transfer as a function of sorbent parameters



# Overview

- Discuss
  - Mass Balance
  - Boundary Conditions
  - Initial Conditions
  - Typical sorbent and model parameters
- Explain Sorbent Size Distribution
- Show Model Results



# Model Development - Mass Balance Equations

Mass balance for a particle:

$$\varepsilon_P \frac{\partial c}{\partial t} = D_{eff} \left( \frac{\partial^2 c}{\partial t^2} + \frac{2}{r} \frac{\partial c}{\partial r} \right) - \rho_P \frac{\partial \omega}{\partial t}$$

where  $c$  represents the gas phase concentration within the particle and  $\omega$  is the solid



# Model Development with Solid Phase Reaction Equation

With rate equation (Scala *et al.*<sup>1</sup>)

$$\varepsilon_P \frac{\partial c}{\partial t} = D_{eff} \left( \frac{\partial^2 c}{\partial t^2} + \frac{2}{r} \frac{\partial c}{\partial r} \right) - \rho_P [k_1 (\omega_{max} - \omega)c - k_2 \omega]$$

With Langmuir equilibrium (Flora *et al.*<sup>2</sup>)

$$\varepsilon_P \frac{\partial c}{\partial t} = \frac{D_{eff} \left( \frac{\partial^2 c}{\partial t^2} + \frac{2}{r} \frac{\partial c}{\partial r} \right)}{1 + \rho_P \left( \frac{\omega_{max} K}{1 + kc} \right) \left( 1 - \frac{Kc}{1 + Kc} \right)} \quad \omega = \frac{\omega_{max} Kc}{1 + Kc}$$

1) F. Scala, *Ind. Eng. Chem. Res.* 43 (2004) 2575 – 2589.

2) J. R. Flora, R. A. Haris, W. J. O'Dowd, H. W. Pennline, R. D. Vidic. *J. Air Waste Manage Assoc.* 43 (2003) 478 – 496.



# Boundary and Initial Conditions

Initial:  $\left. \frac{\partial c}{\partial r} \right|_{r=0,T} = 0 \quad c(r,0) = 0 \quad c_b(0) = c_b^\circ \quad \omega(r,0) = 0$

Surface:  $\left. \frac{\partial c}{\partial r} \right|_{r=R_p,t} = \frac{k_f}{D_{eff}} (c_b(t) - c(R_p, t))$

Bulk:  $\frac{\partial c_b}{\partial t} = - \frac{3F_{feedrate} D_{eff}}{\rho_p R_p} \left. \frac{\partial c}{\partial r} \right|_{r=R_p,t}$

Coefficients:  $D_{kn} = 9700 r_{pore} \left( \frac{T}{M_A} \right)^{1/2} \quad D_{eff} = \frac{\varepsilon_p}{\tau_p} \left( \frac{1}{D_{kn}} + \frac{1}{D_m} \right)^{-1}$

$$k_f = \frac{D_m Sh}{2R_p}$$

Add more about the parameters

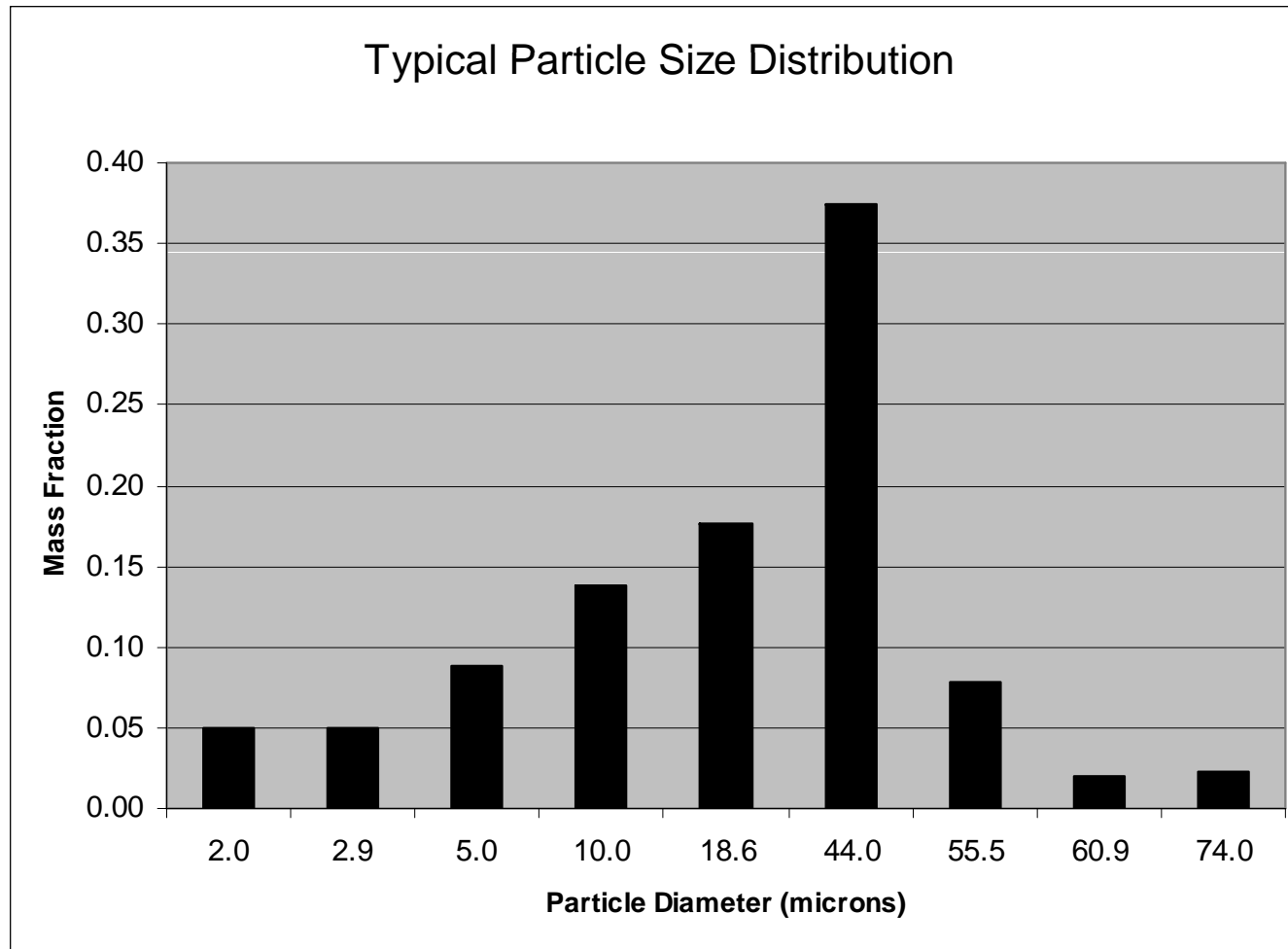


# Sorbent Parameters

<i>Sorbent</i>	<i>T</i> (°C)	<i>k</i> <sub>1</sub> (m <sup>3</sup> /g/s)	<i>k</i> <sub>2</sub> (1/s)	<i>K</i> (m <sup>3</sup> /g)	<i>ω</i> <sub>max</sub> (g / g)	<i>D</i> <sub>eff</sub> (m <sup>2</sup> /s)
HGR	120	0.41	7.06E-04	5.81E+02	8.20E-04	6.46E-07
<i>D</i> <sub>kn</sub> (m <sup>2</sup> /s)	<i>D</i> <sub>m</sub> (m <sup>2</sup> /s)	<i>C</i> <sub>b</sub> <sup>o</sup> (ug /m <sup>3</sup> )	<i>Feed</i> <i>Rate</i> (g / m <sup>3</sup> )	<i>ε</i> <sub>P</sub>	<i>ρ</i> <sub>P</sub> (kg/m <sup>3</sup> )	<i>Pore</i> <i>Size</i> (nm)
1.97E-06	2.45E-05	5.0	10	0.50	990	30



# Sorbent Parameters: Average Particle Diameter: 29.6 $\mu\text{m}$

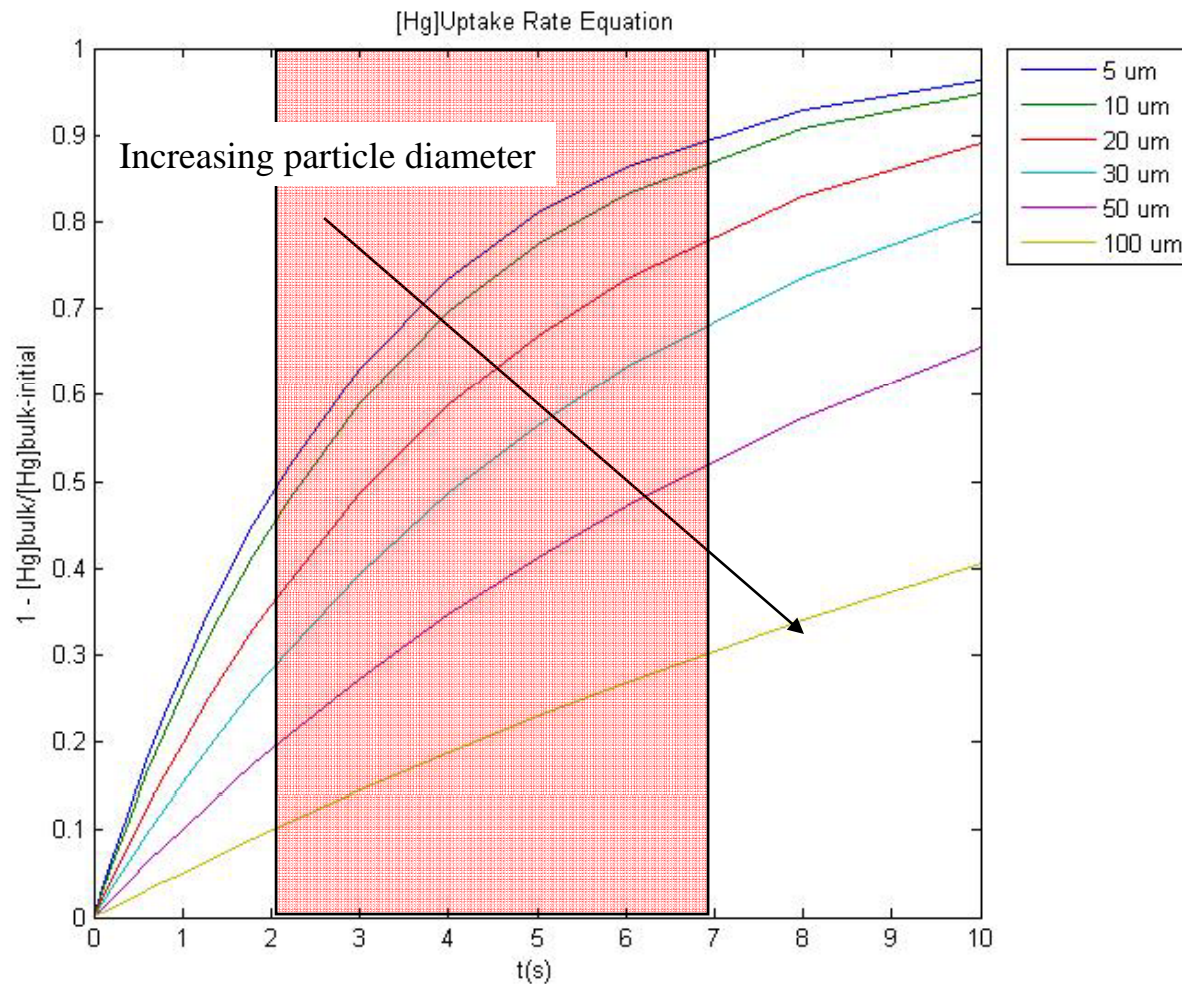




# Model Results: Hg Removal versus time

Using rate equation and feed rate = 10 g Sorbent / g flue gas

As particle diameter increases, uptake decreases

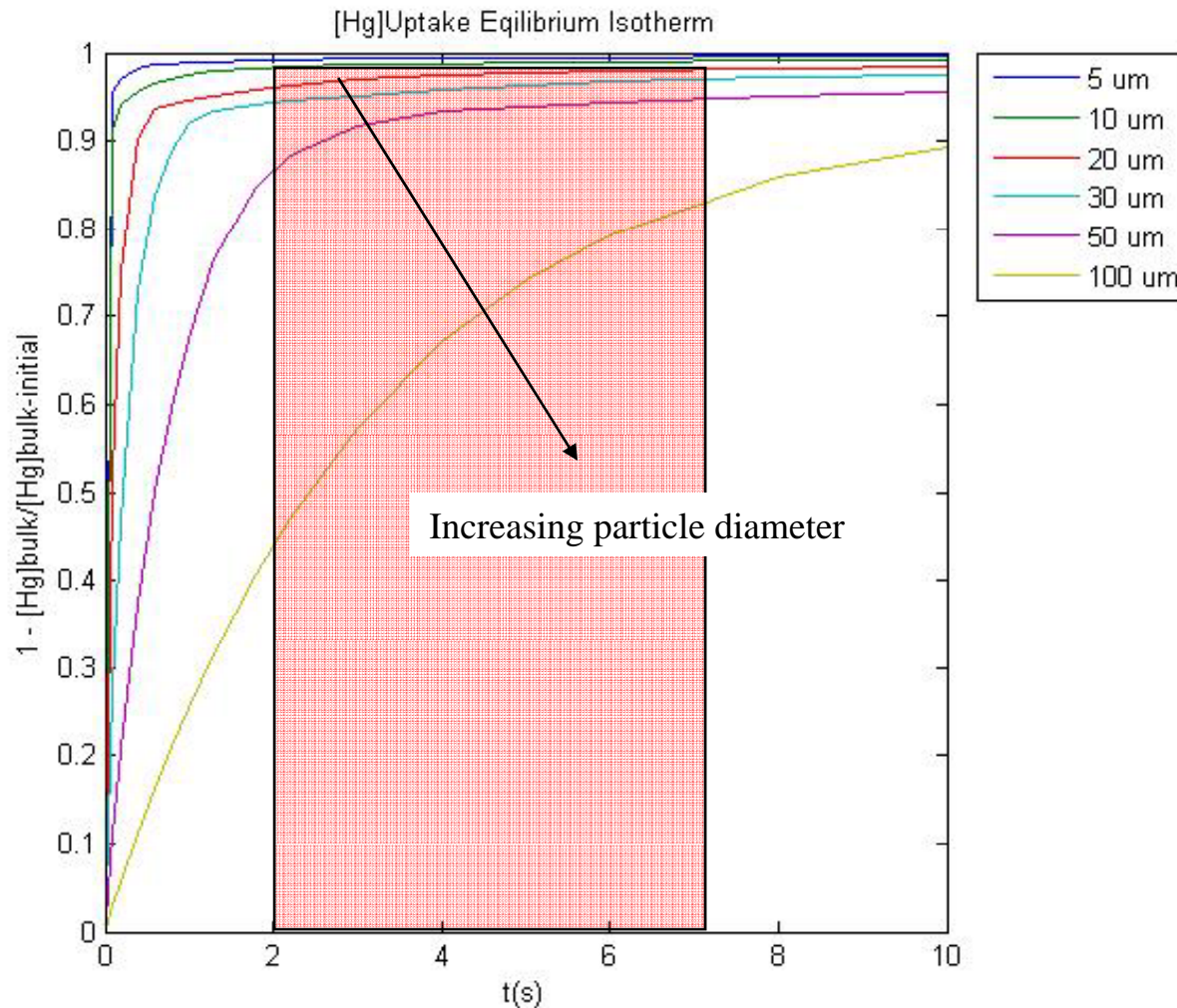




# Model Results: Hg Removal versus time

Using equilibrium and feed rate = 10 g Sorbent / g flue gas

As particle diameter increases, uptake decreases

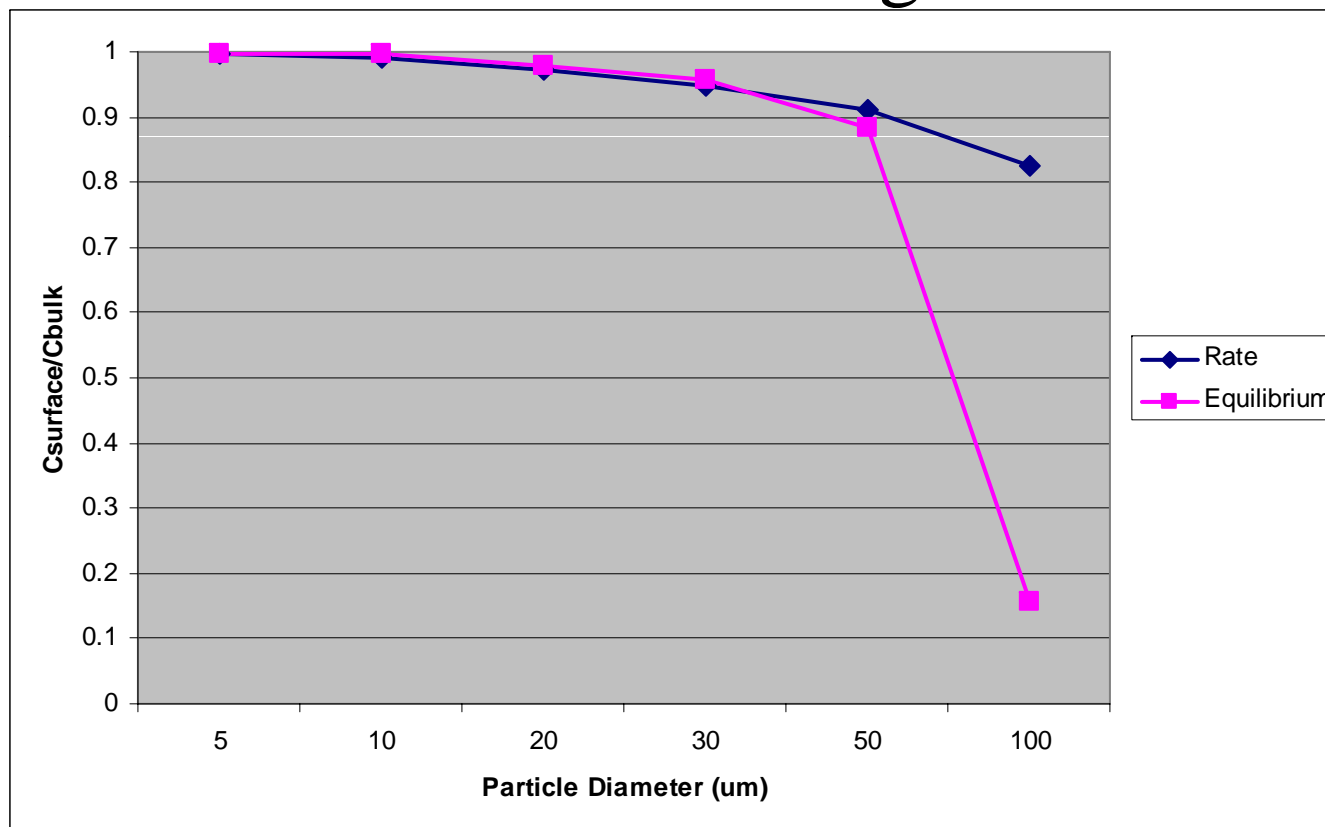




# Model Results: Hg Uptake at 4 seconds.

As particle diameter increases, external mass transfer resistance also increases.

Feed rate =  $10 \text{ g/m}^3$

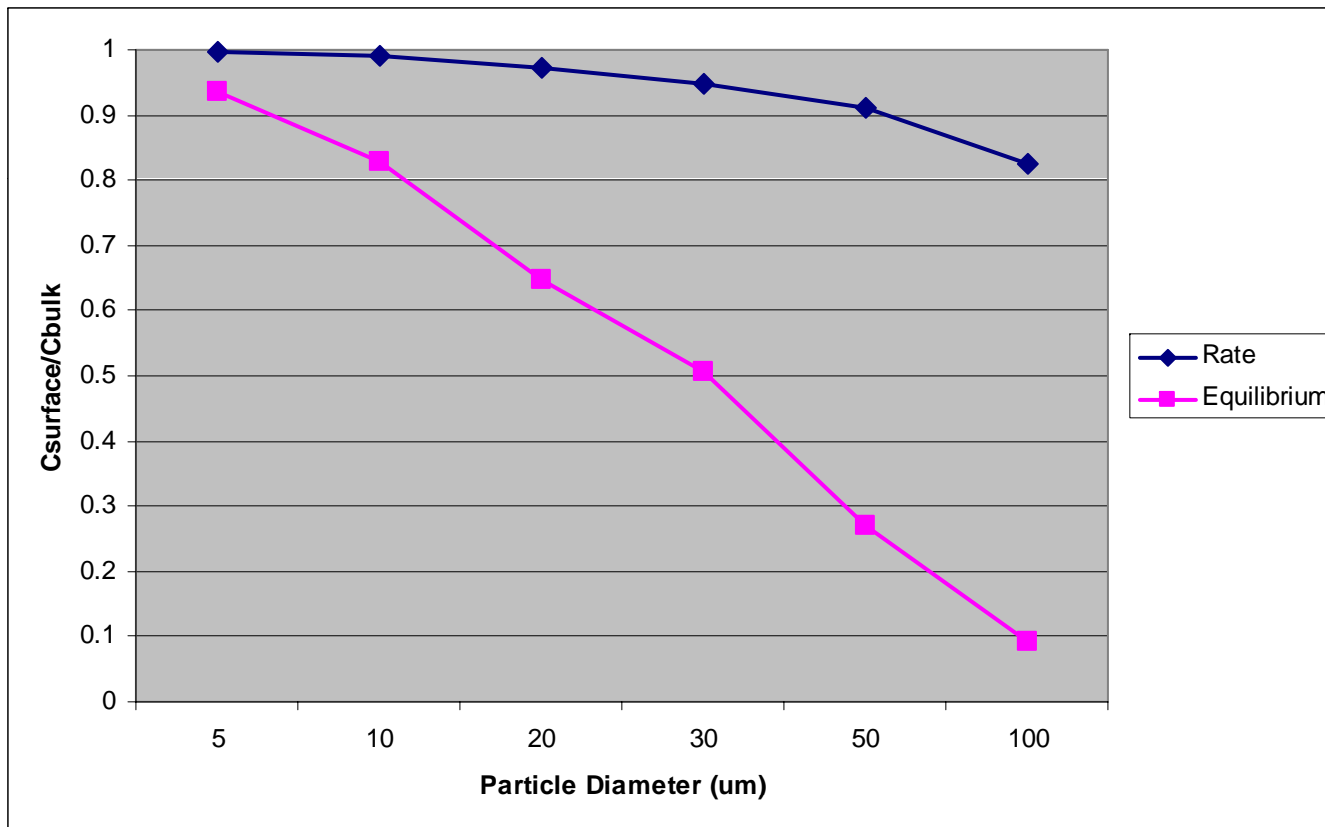




# Model Results: Hg Uptake at 4 seconds.

As particle diameter increases, external mass transfer resistance also increases.

Feed Rate:  $0.1 \text{ g/m}^3$

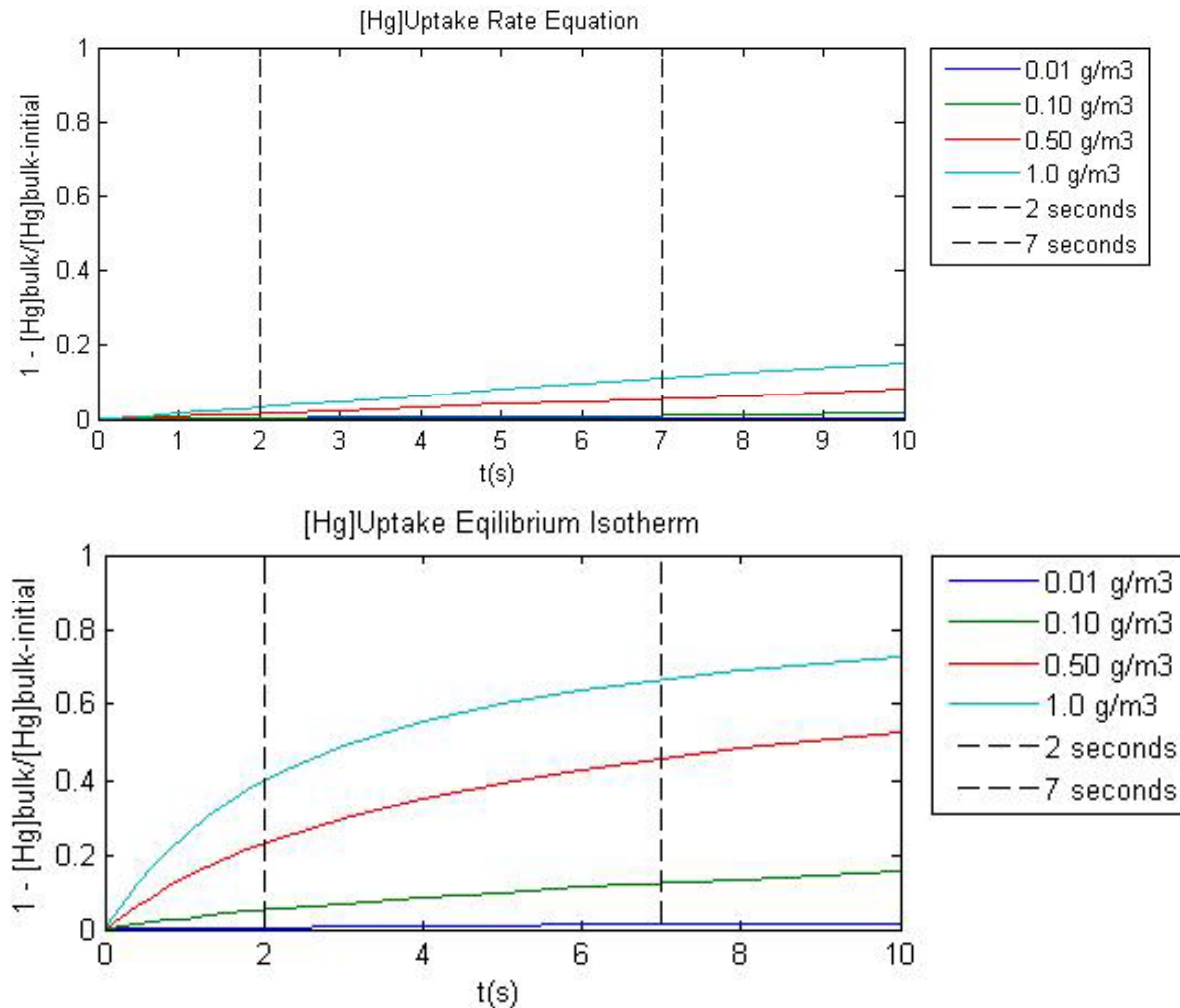




# Rate vs Equilibrium with variable feed rate.

Particle Diameter:  $30\ \mu\text{m}$

## More Hg is absorbed using equilibrium assumption





# Conclusions

- External mass transfer is minimized with sorbent particles  $< 20 \text{ um}$
- Sorbent parameters and feeding rate are crucial in the optimization of mercury uptake.
- Even with high feeding rates and high uptake potentials, in flight adsorption will rarely exceeded 30%
  - Further removal mechanisms, such as packed bed adsorption, are likely taking place in full scale systems



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