Recycle Process Development and Simulation

(Subtask C-3-1)

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Objectives:

- Simulating the fundamentals of UPW systems with and without recycle (Design for Environment tool).
- Utilizing the simulator to understand the dynamics of impurity distribution.
- Utilizing the simulator to develop novel recycle strategies and configurations.
- Integrated rinse and recycle simulation and optimization
- Metrology and control tools and techniques for advanced future UPW systems.

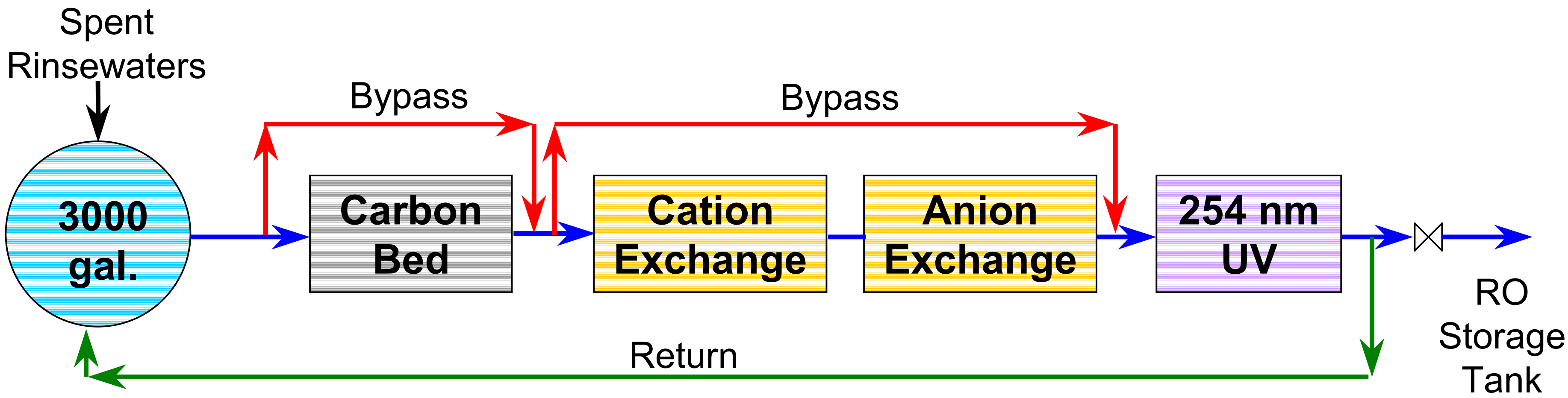
ESH Impact:

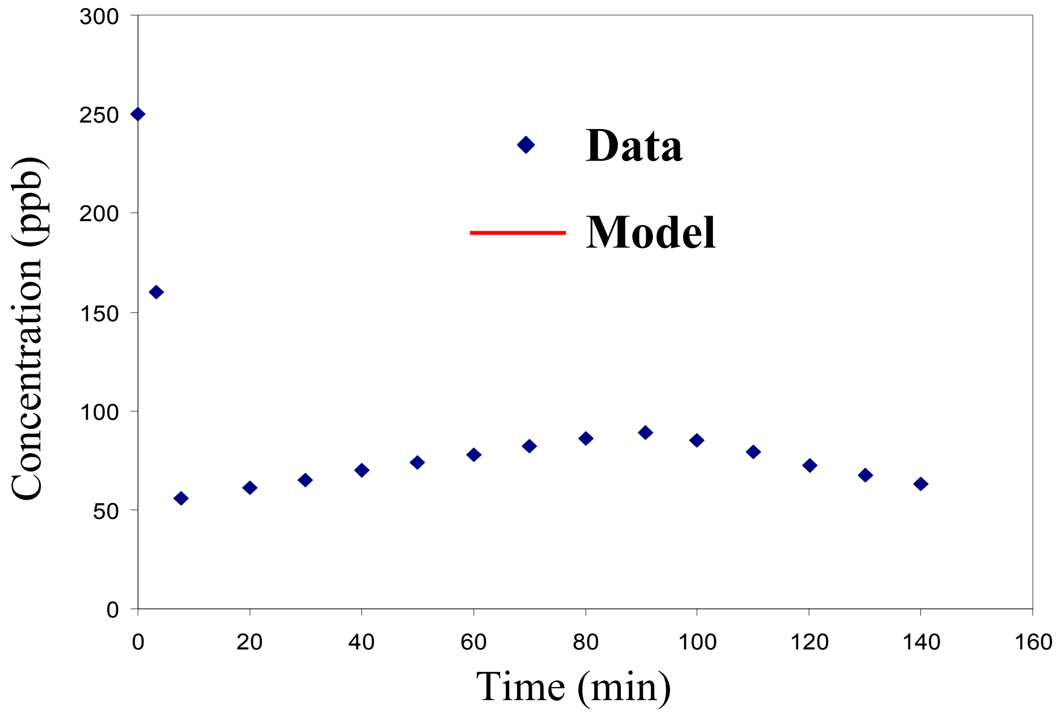
- Increased water recycling is a critical requirement in future fabs.
- This technology will facilitate low-risk and low-cost water recycling.

Method of Approach:

- Part 1: Data base on process module fundamentals.
- Part 2: Development of the simulation theory and computational codes.
- Part 3: Application and validation.

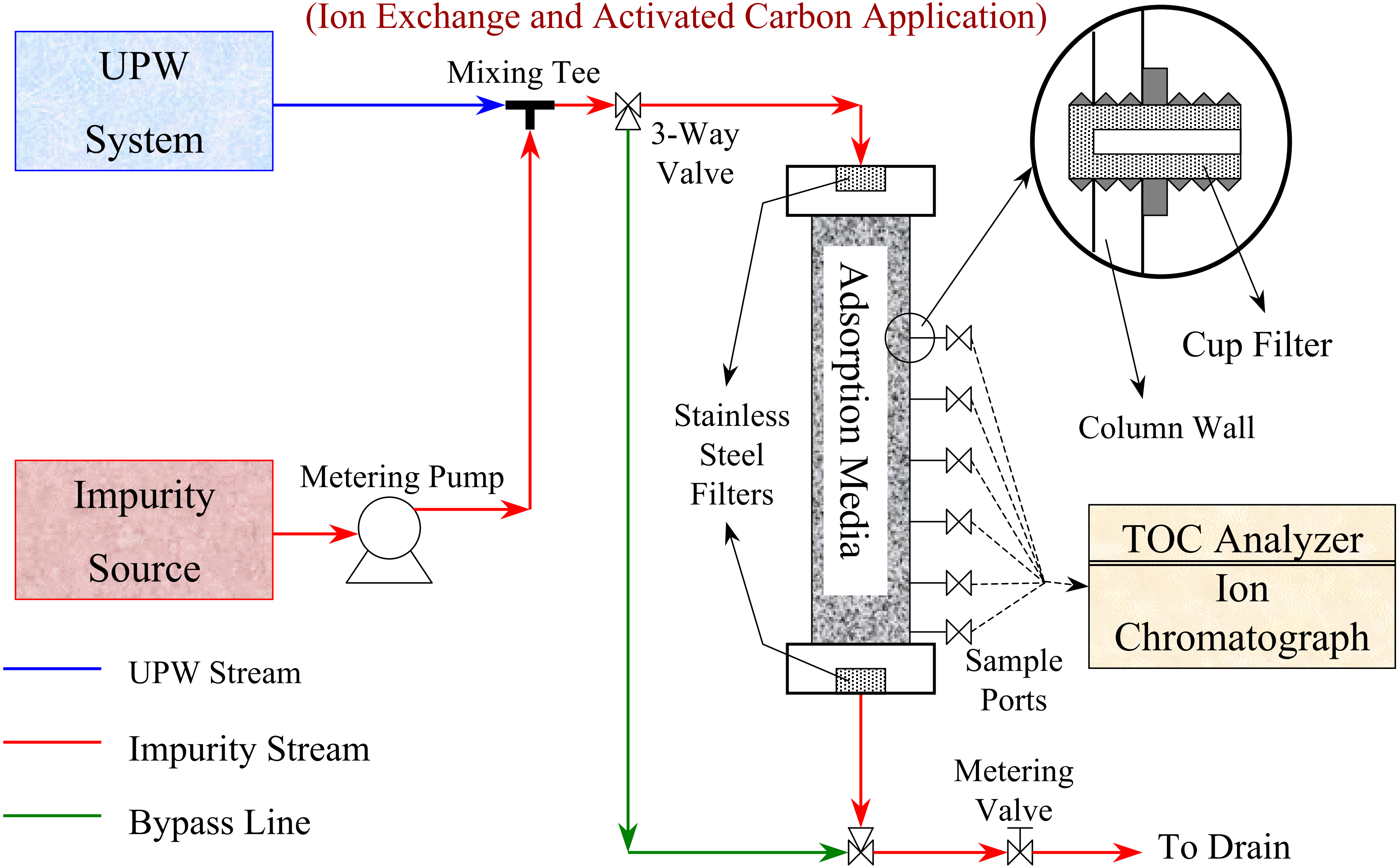
Member Company Recycle System with IPA





Experimental Setup for Adsorption Studies

(Ion Exchange and Activated Carbon Application)



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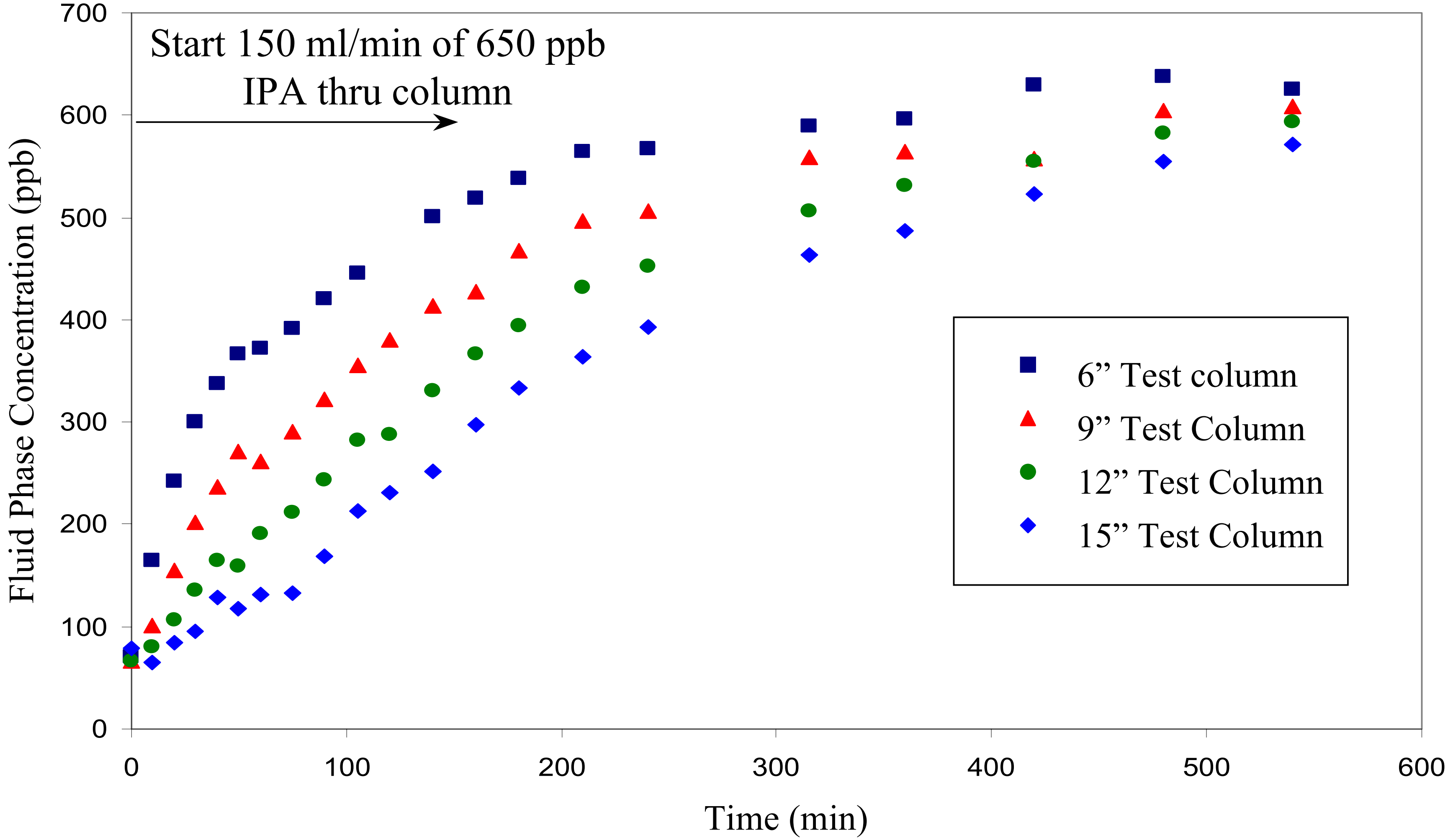
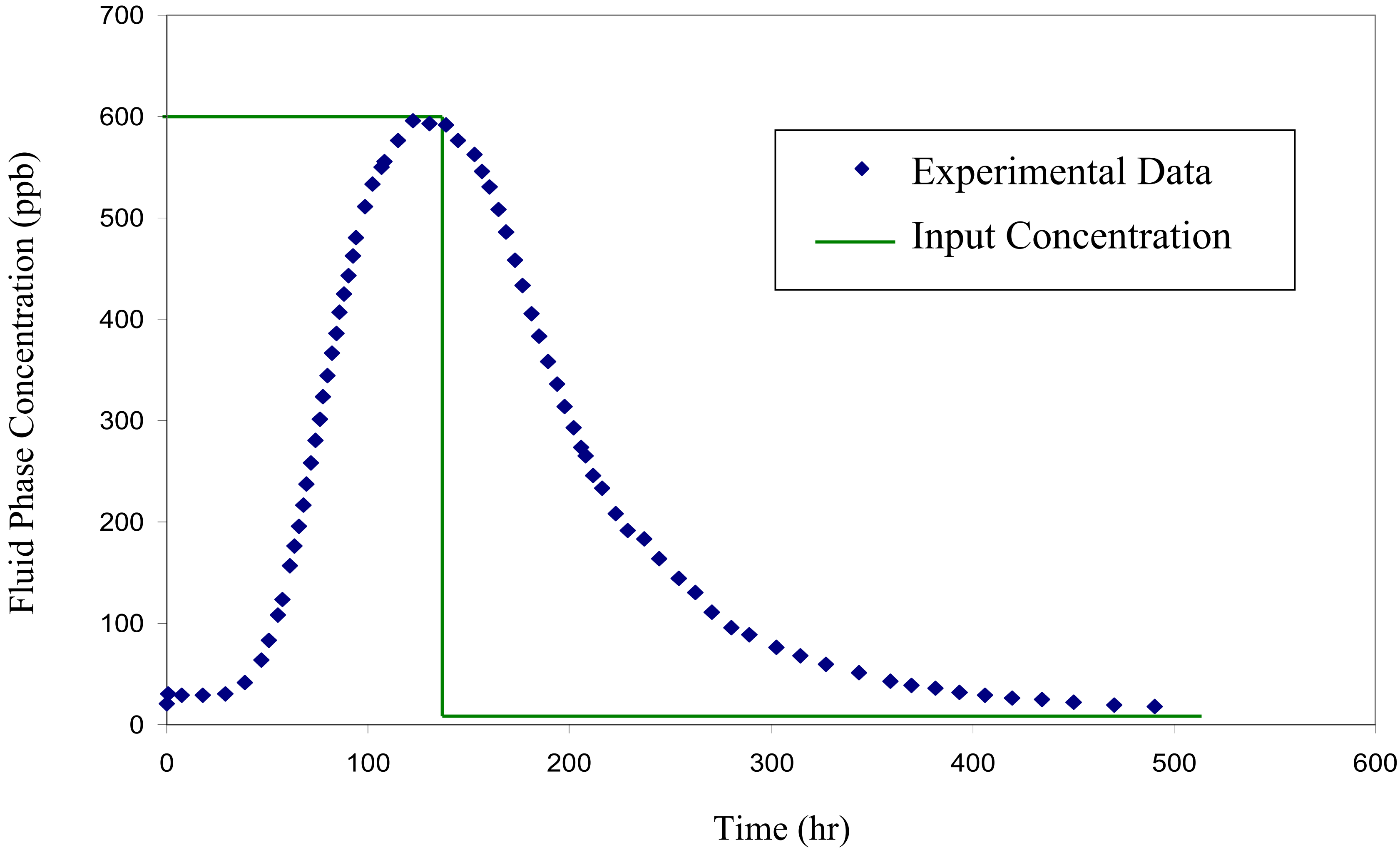
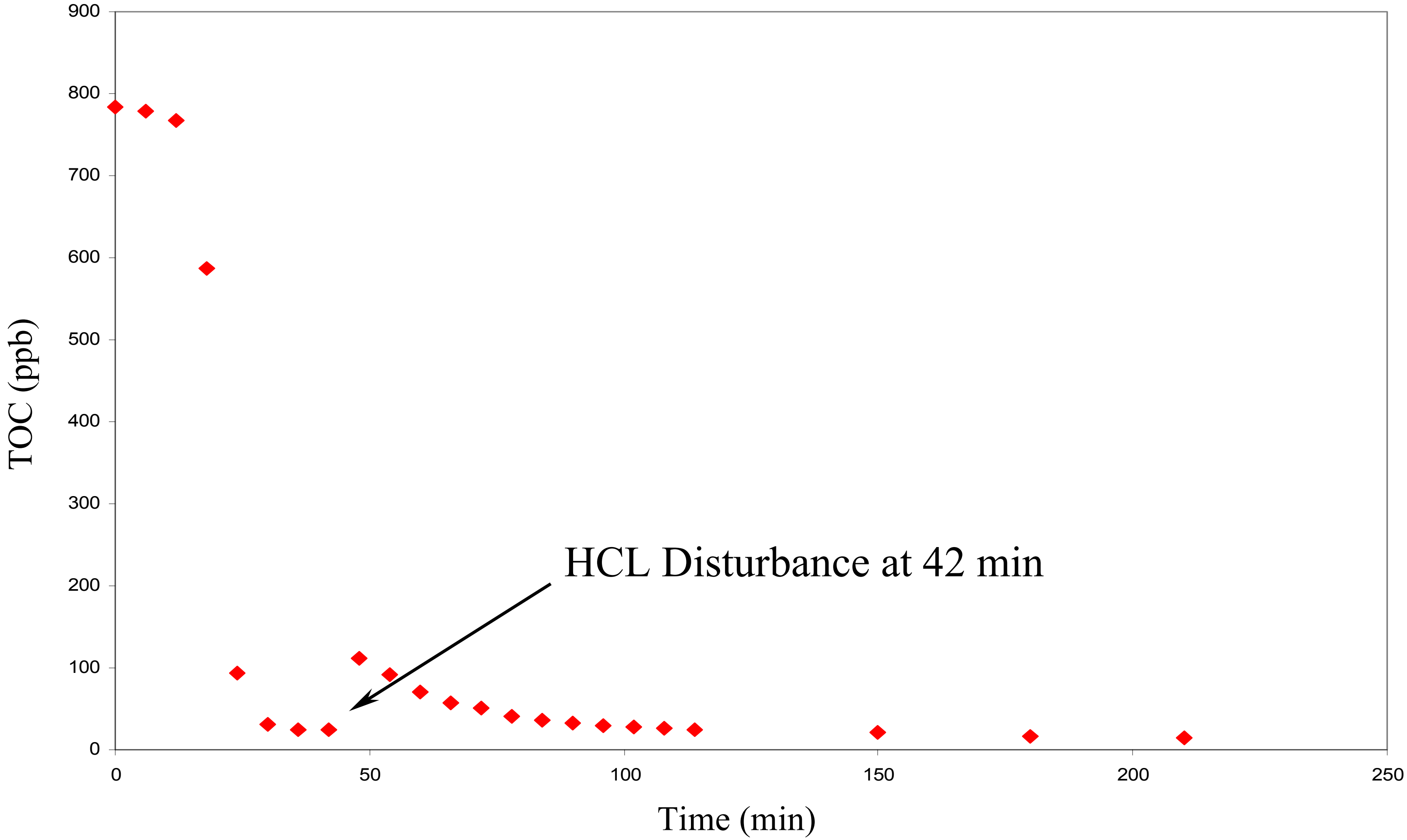
Adsorption of IPA on Coconut Shell Activated Carbon



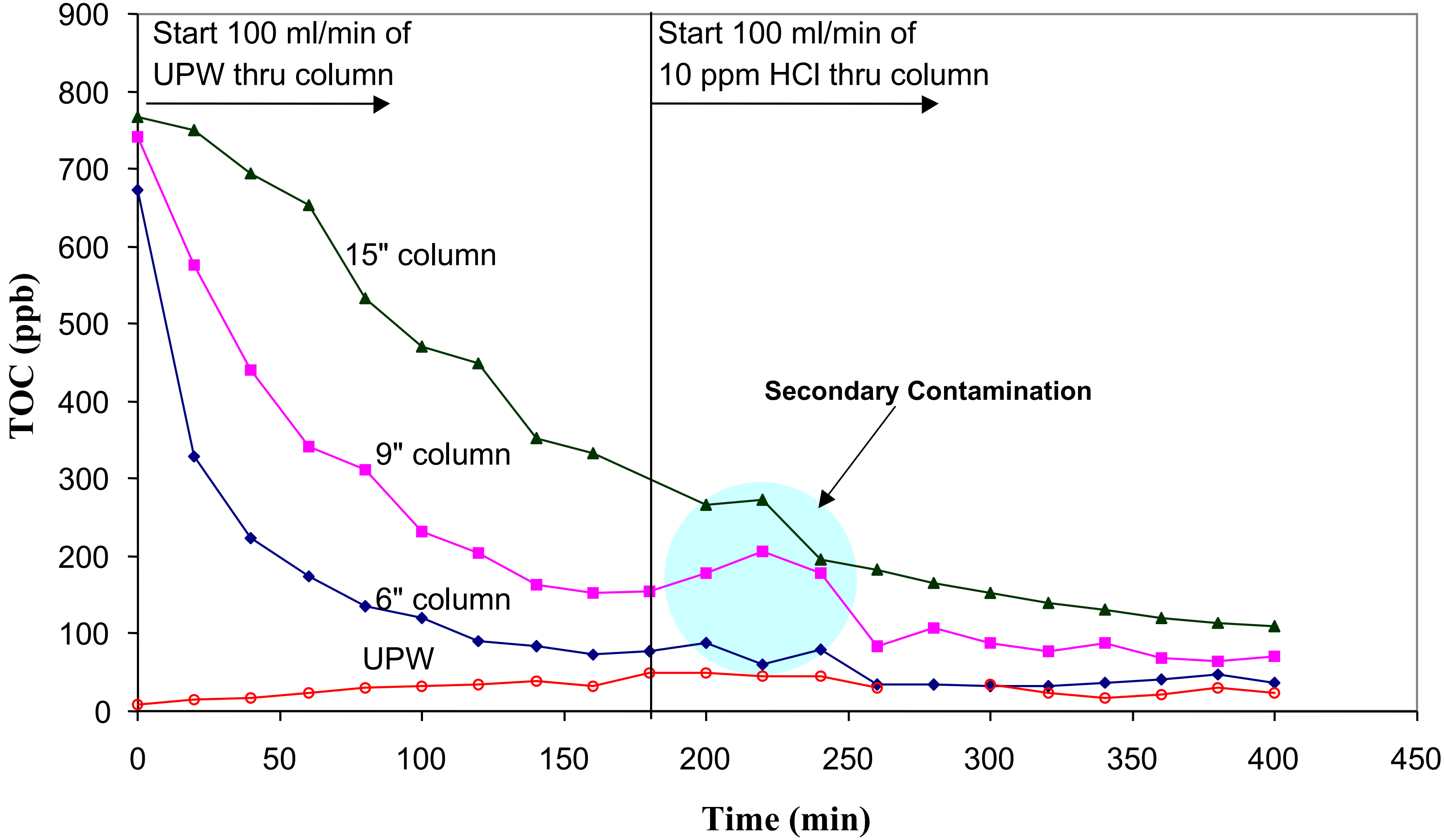
Adsorption/Desorption of $CHCl_3$ on Coconut Shell Activated Carbon



Effect of HCl on the Leakage of Ethylene Glycol from Activated Carbon



Secondary Contamination due to Desorption of IPA from Activated Carbon



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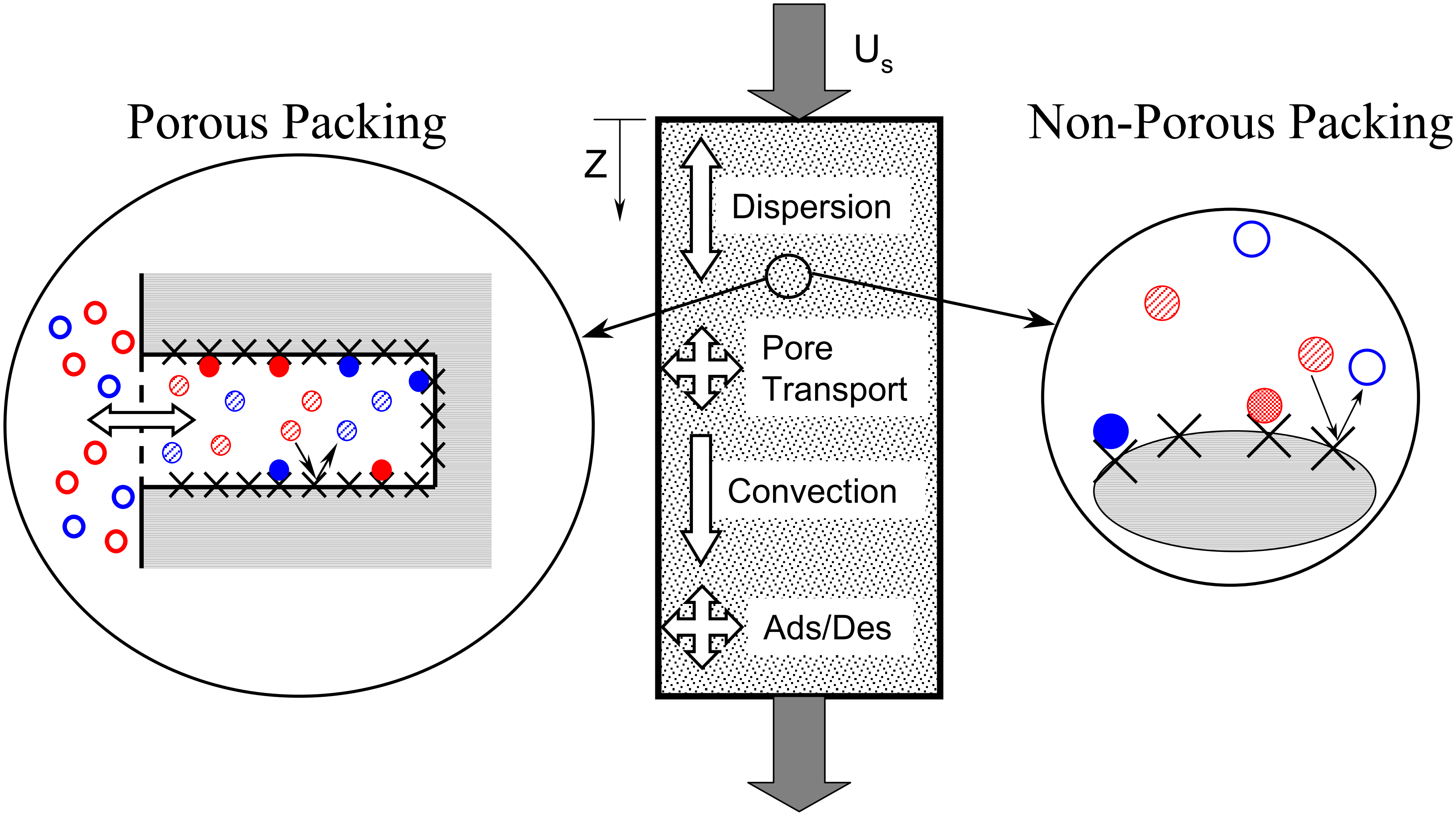
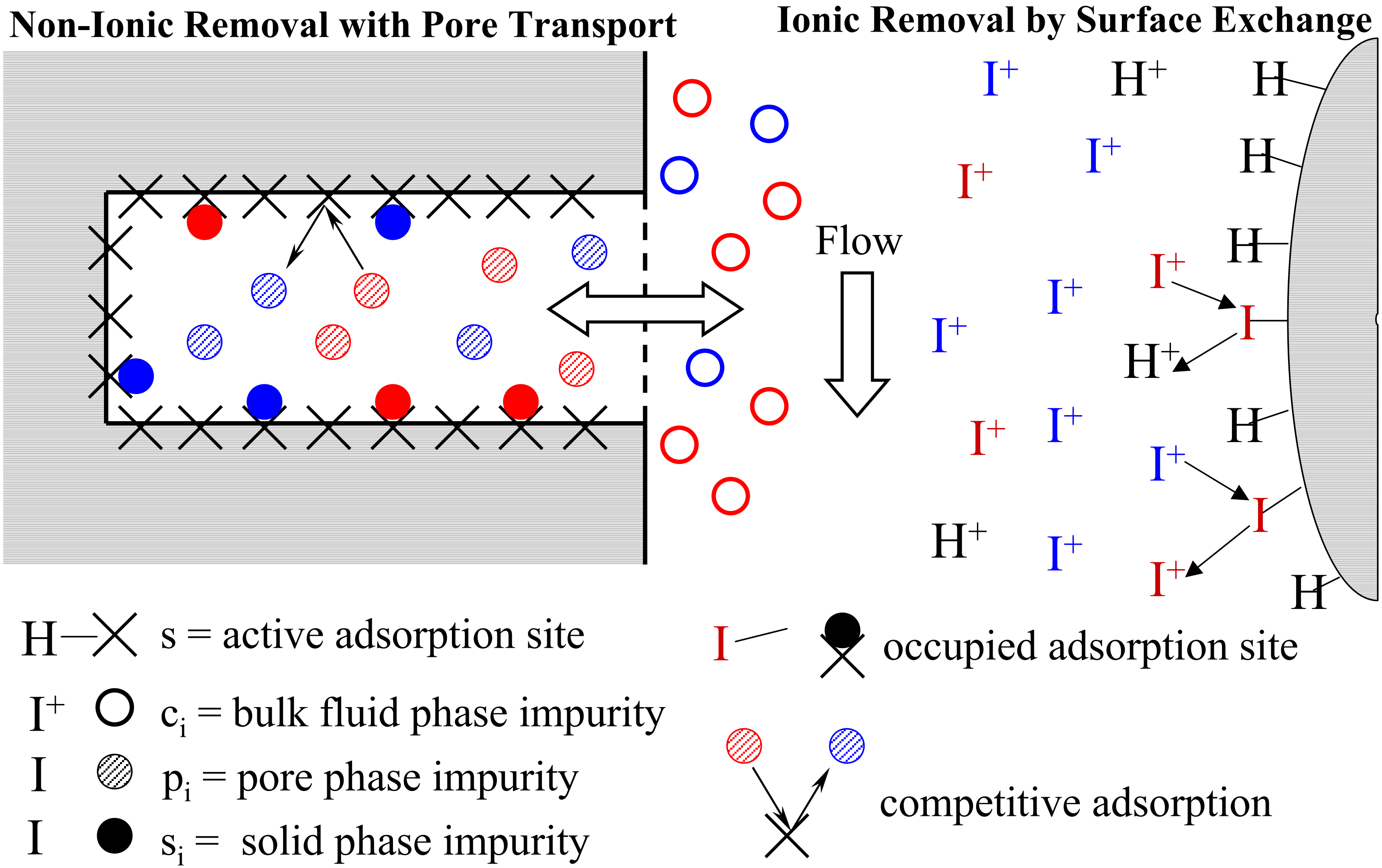
Transport Processes in Packed Bed Reactors



Dynamics of Multi-component Impurity Removal by Adsorption



Multi-component Model for Adsorption Processes

Non-Porous Adsorption Media

Local Reaction:

$$I_i \; + \; X \; \leftrightarrow \; I_i \cdot X$$

Adsorbed Phase Conservation:

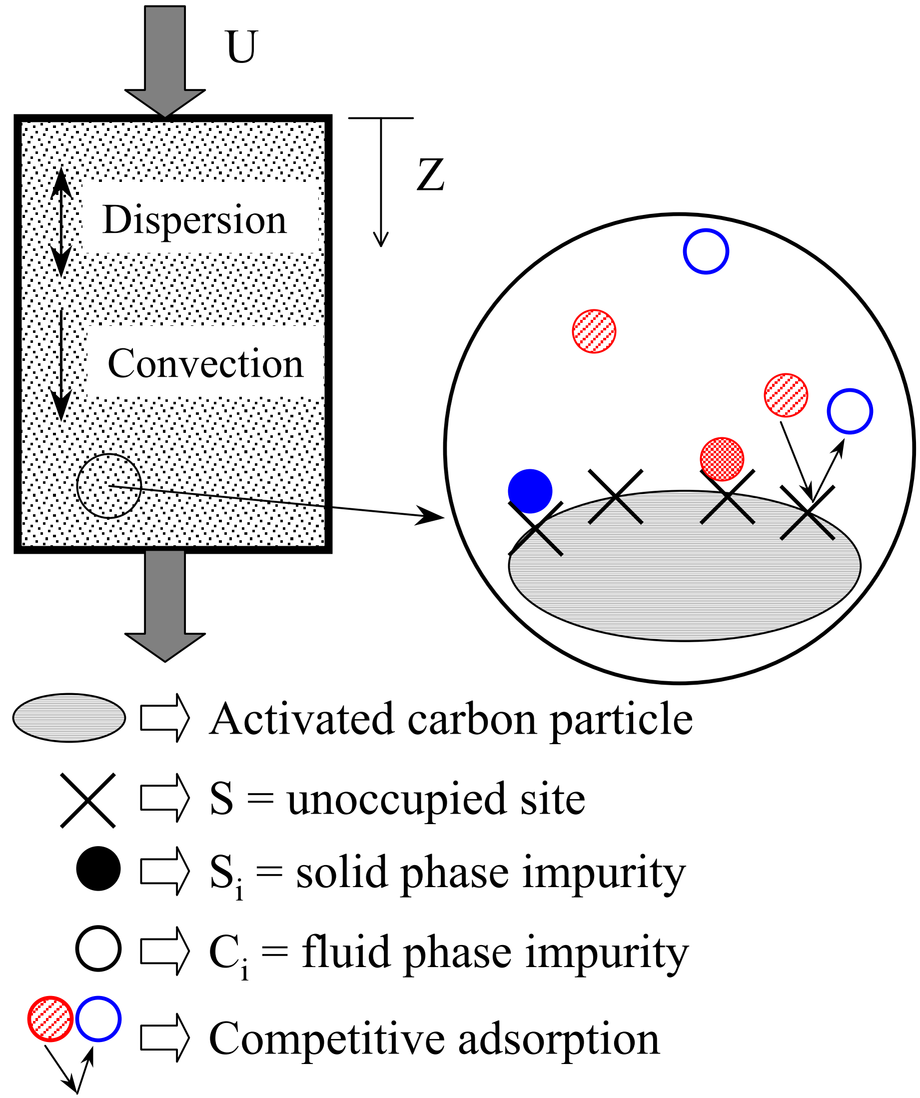
$$\frac{\partial s_i}{\partial t} = k_{ai} c_i \left(\frac{s}{1+as_i} \right) - k_{di} \left(\frac{s_i}{1+as_i} \right)$$

Fluid Phase Conservation:

$$\varepsilon \frac{\partial c_i}{\partial t} - (1-\varepsilon) \frac{\partial s_i}{\partial t} = -U\varepsilon \frac{\partial c_i}{\partial z} + D\varepsilon \frac{\partial^2 c_i}{\partial z^2}$$

Sites Conservation:

$$s_o = s + \sum_i s_i$$



Multi-component Model for Adsorption Processes

Porous Adsorption Media

Adsorbed Phase Conservation:

$$\frac{\partial s_i}{\partial t} = k_{ai}\, p_i \left(\frac{s}{1 + a\, s_i} \right) - k_{di} \left(\frac{s_i}{1 + a\, s_i} \right)$$

Pore Phase Conservation:

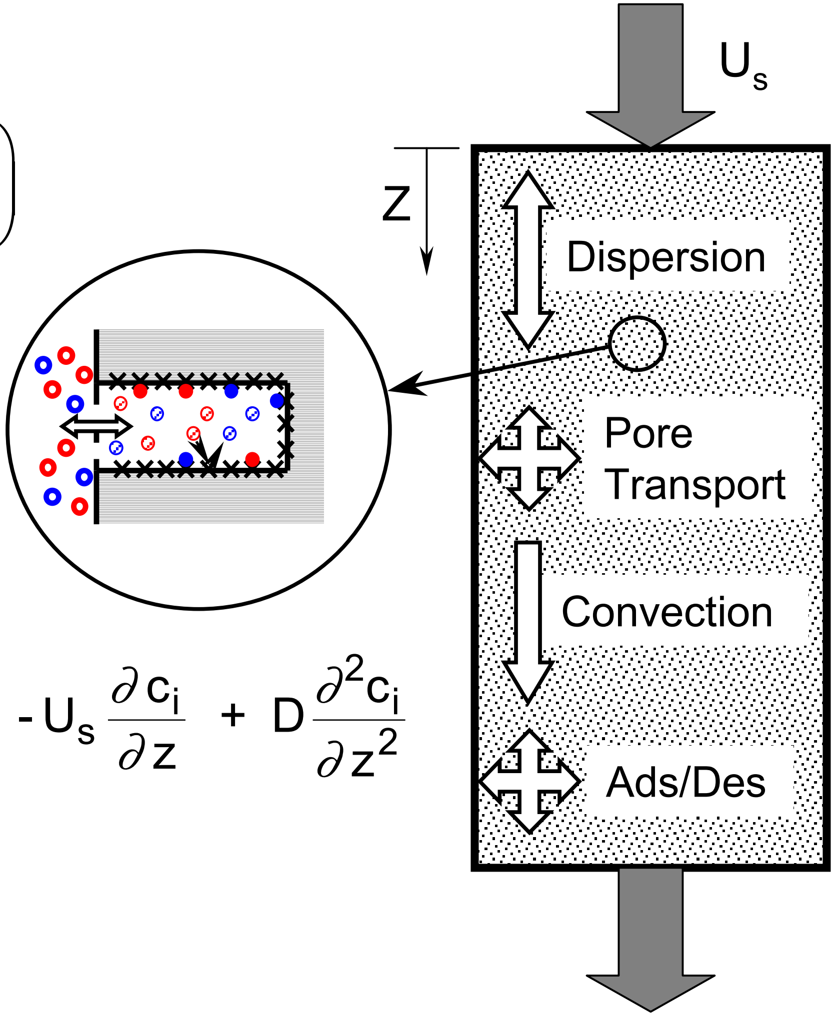
$$\varepsilon_p \frac{\partial p_i}{\partial t} + \frac{\partial s_i}{\partial t} = \alpha\, k_{pi} (c_i - p_i)$$

Bulk Fluid Phase Conservation:

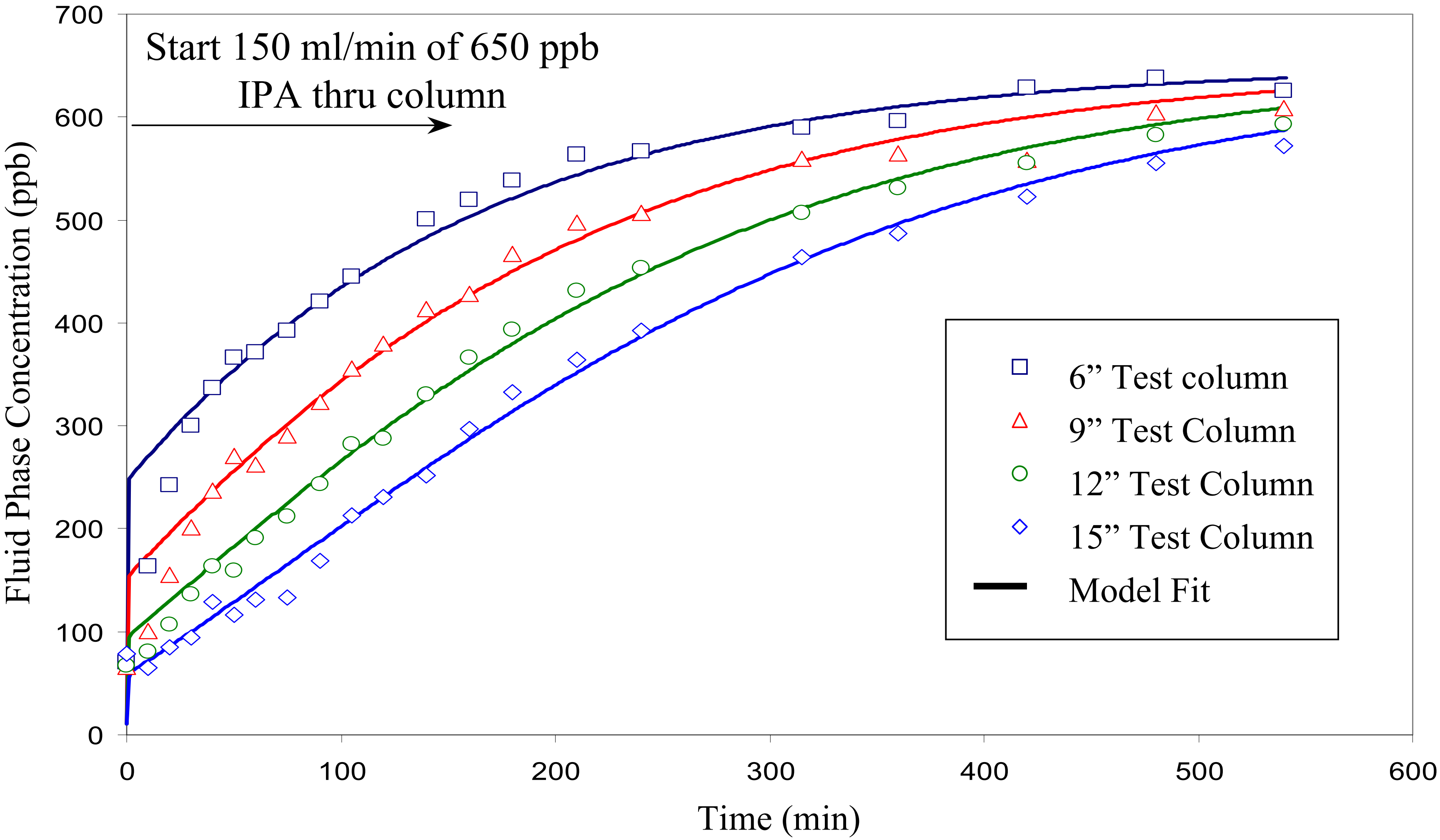
$$\varepsilon_b \frac{\partial c_i}{\partial t} + \varepsilon_p (1 - \varepsilon_b) \frac{\partial p_i}{\partial t} + (1 - \varepsilon_b) \frac{\partial s_i}{\partial t} = -U_s \frac{\partial c_i}{\partial z} + D \frac{\partial^2 c_i}{\partial z^2}$$

Sites Conservation:

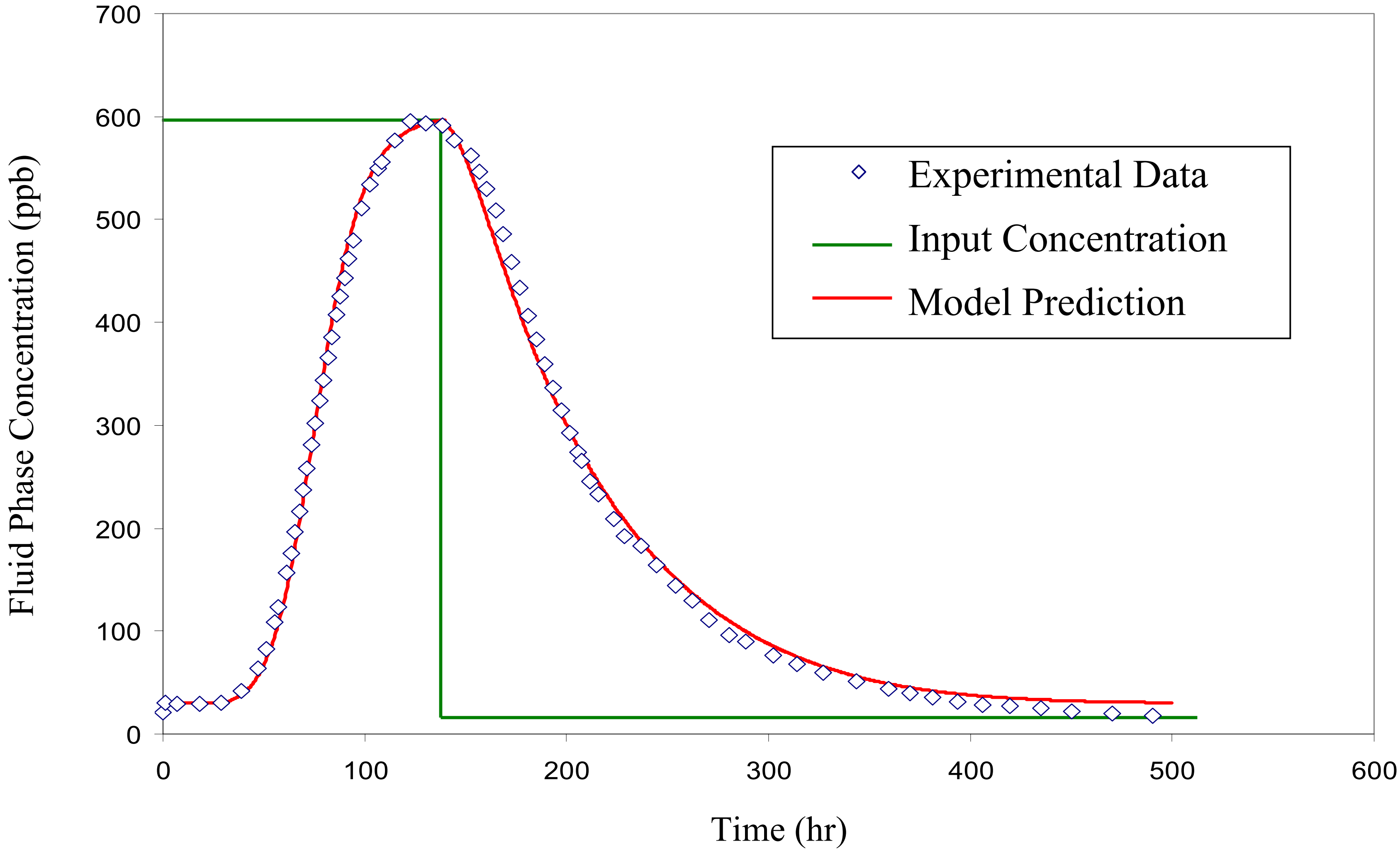
$$s_o = s + \sum_i s_i$$



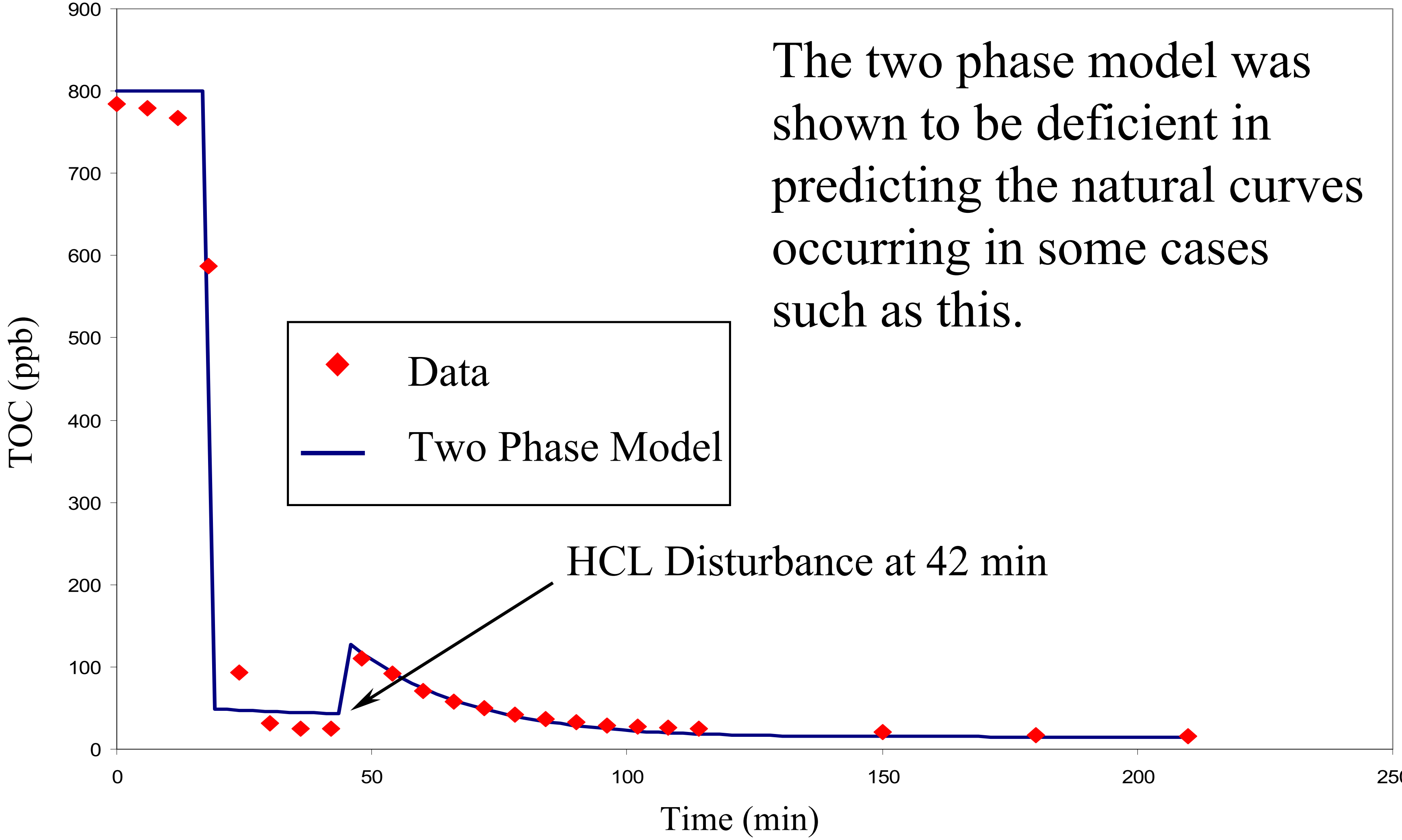
Adsorption of IPA on Coconut Shell Activated Carbon



Adsorption/Desorption of $CHCl_3$ on Coconut Shell Activated Carbon

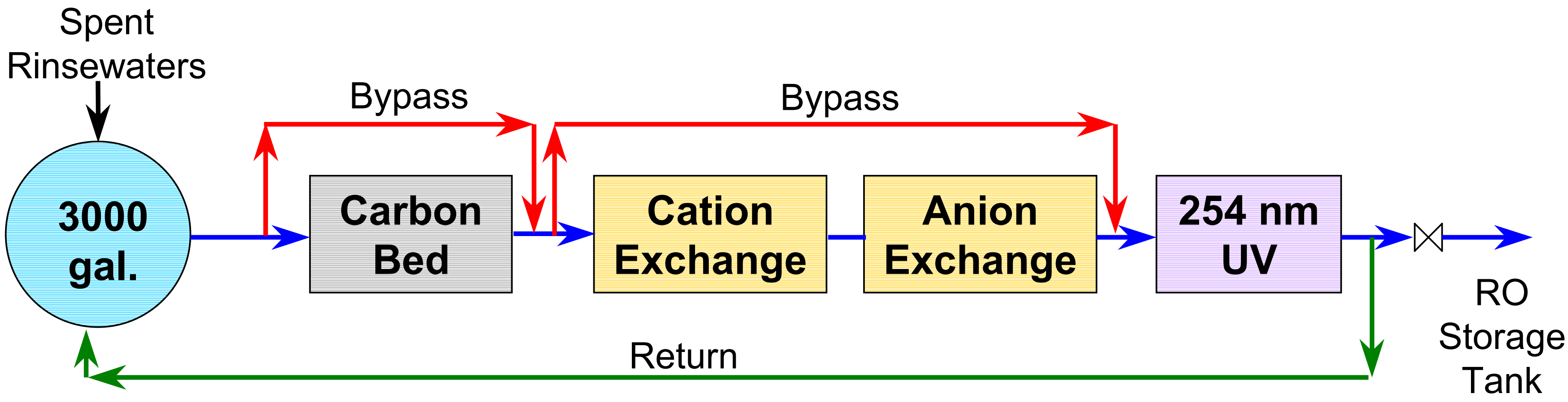


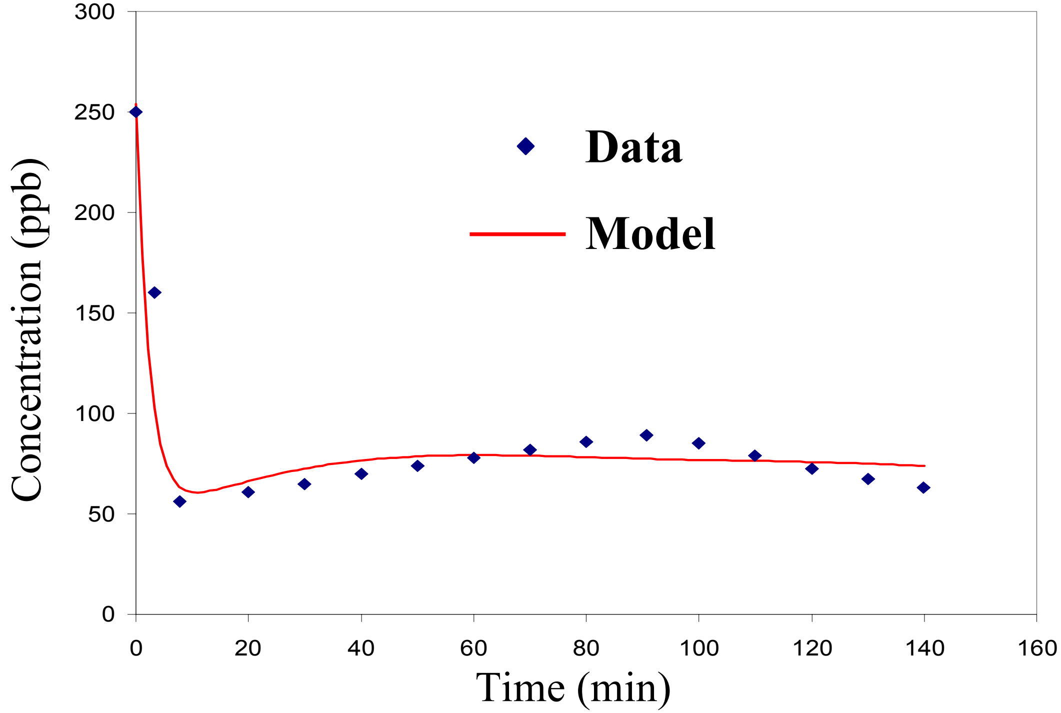
Effect of HCl on the Leakage of Ethylene Glycol from Activated Carbon



The two phase model was shown to be deficient in predicting the natural curves occurring in some cases such as this.

Member Company Recycle System with IPA

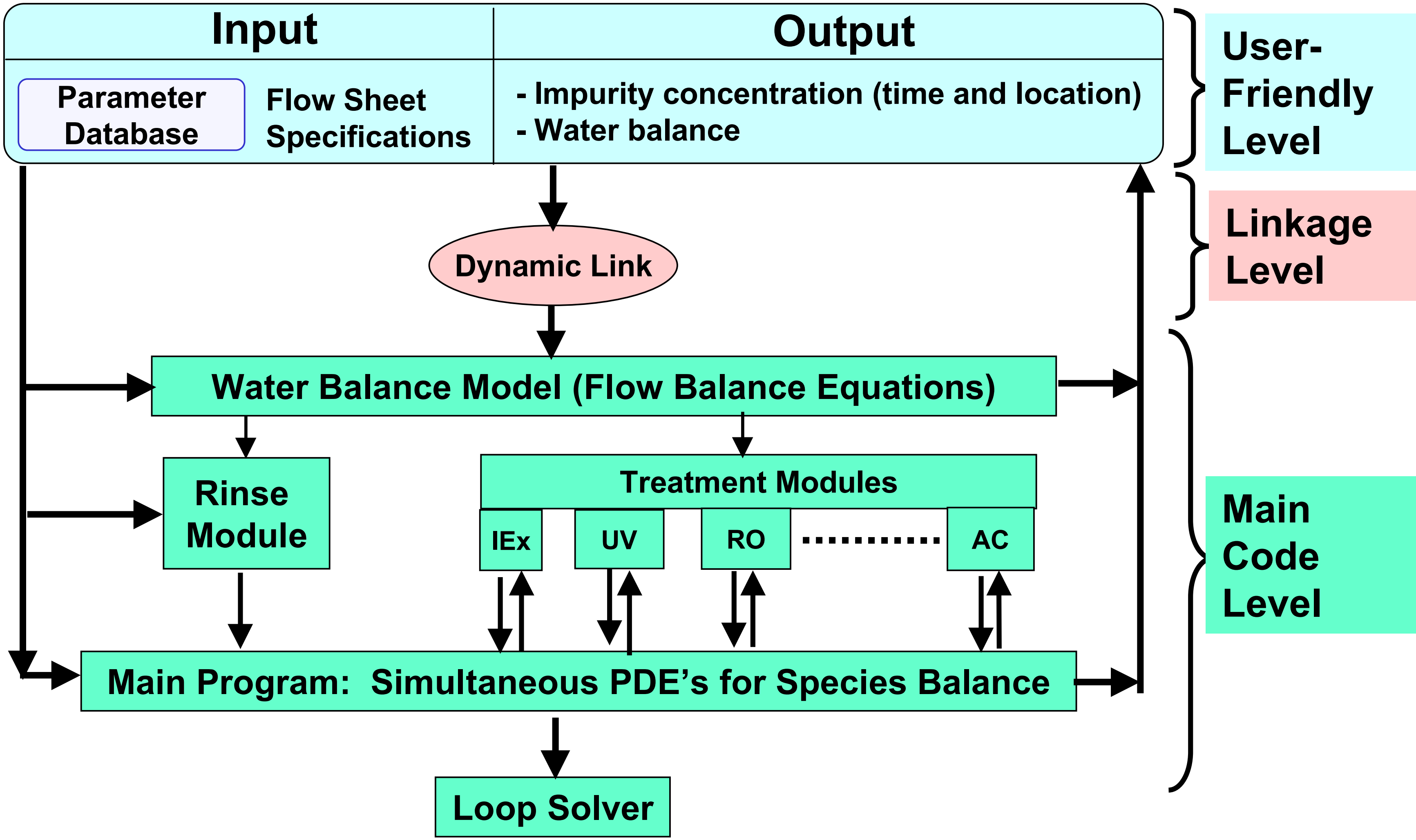




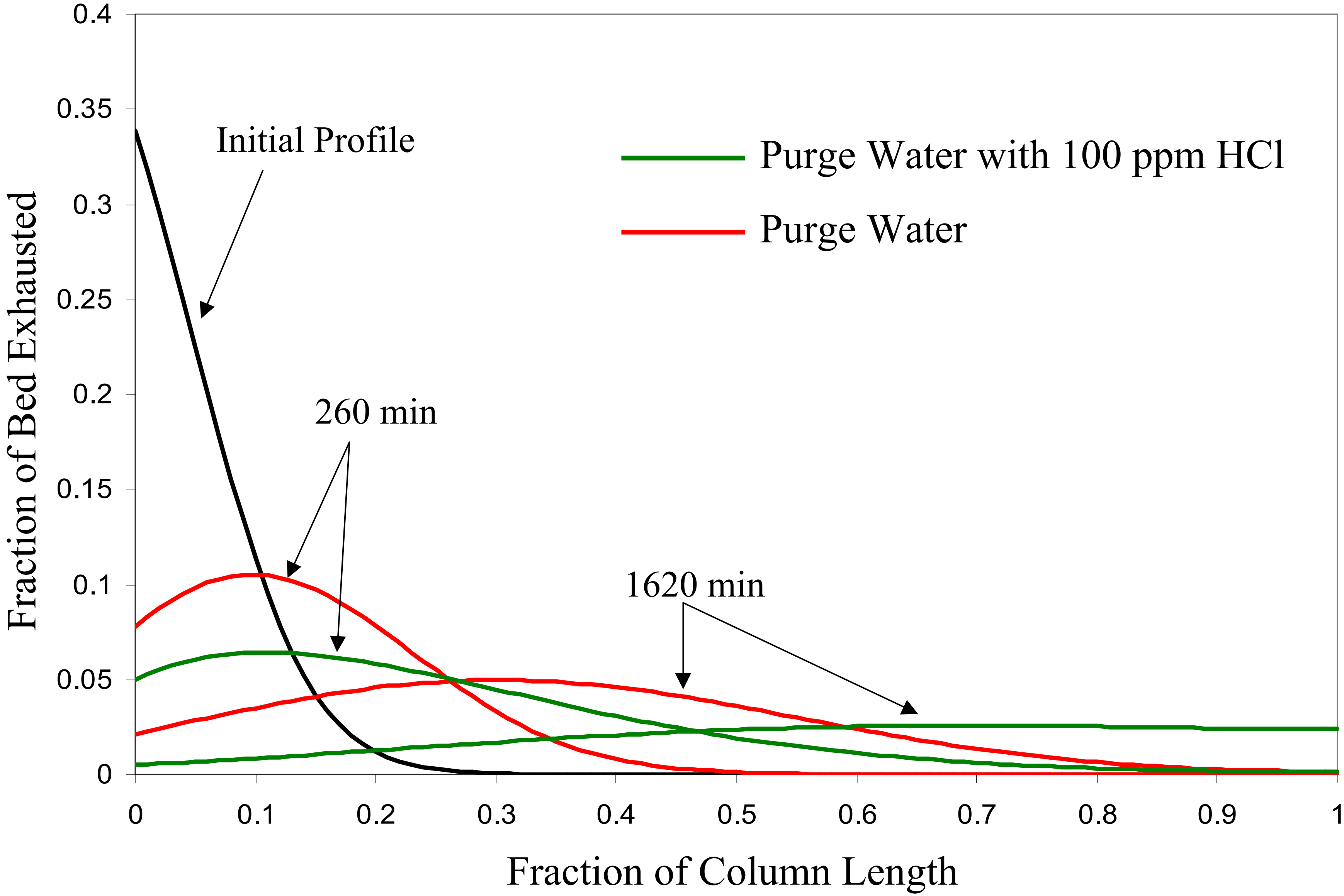
Kinetic Parameters for Various Organic Impurities

Test Compound	AC Type	Capacity, So moles sites/cm^3	$k_{adsorption}$ cm^3/moles C min	$k_{desorption}$ min^{-1}
IPA	Calgon PCB	3.1×10^{-5}	4.3×10^{4}	8.3×10^{-3}
$CHCl_3$	Calgon PCB	1.7×10^{-4}	4.8×10^{4}	1.7×10^{-3}
Ethylene Glycol	Calgon PCB	2.0×10^{-5}	1.0×10^{5}	1.3×10^{-2}
Ethylene Glycol + HCl	Calgon PCB -	2.0×10^{-5} -	2.3×10^{6} -	1.0×10^{-1} -
FC-93	Calgon PCB	4.0×10^{-5}	1.5×10^{5}	2.5×10^{-2}
FC-93	Calgon F-400	4.0×10^{-5}	1.5×10^{5}	3.0×10^{-2}

Structure of the UPW Recycle Simulator

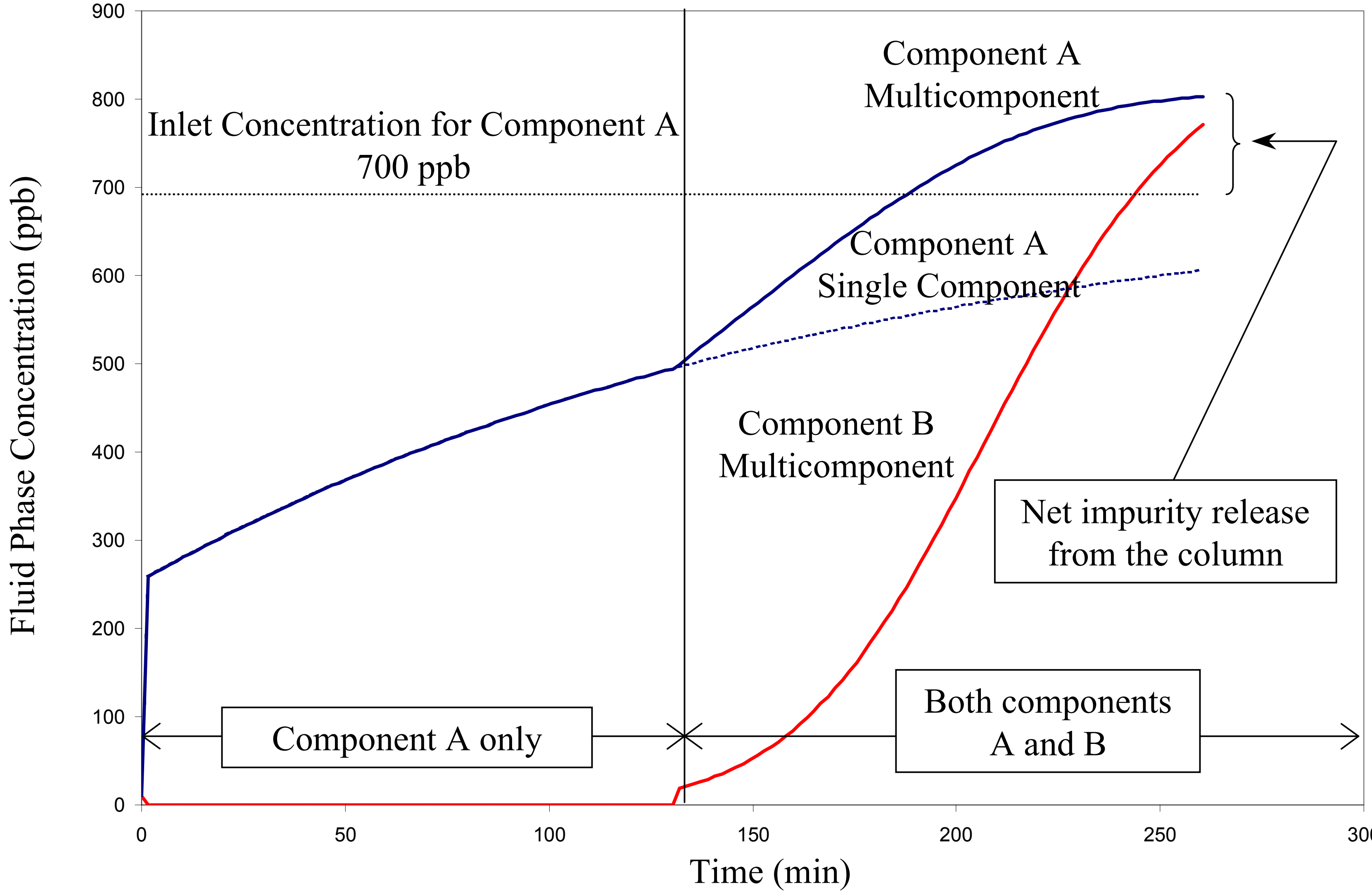


Ethylene Glycol Elution from Activated Carbon



Impurity Release due to Multicomponent Interaction

(Adsorption on Activated Carbon)



Conclusions and Highlights

- The multi-component formulation of adsorption/desorption processes (carbon bed, ion exchange) is nearly completed. The new formulation allows for pore effects, surface interactions and competitive adsorption and desorption.
- Experiments were conducted to determine the fundamental kinetic parameters for adsorption/desorption of model compounds.
- Determined the underlying mechanism of secondary contamination in ion exchange and carbon bed units used for recycle treatment.
- Worked with industry on validation and application of the new simulator.