Application of Simulation in UPW Preparation and Distribution

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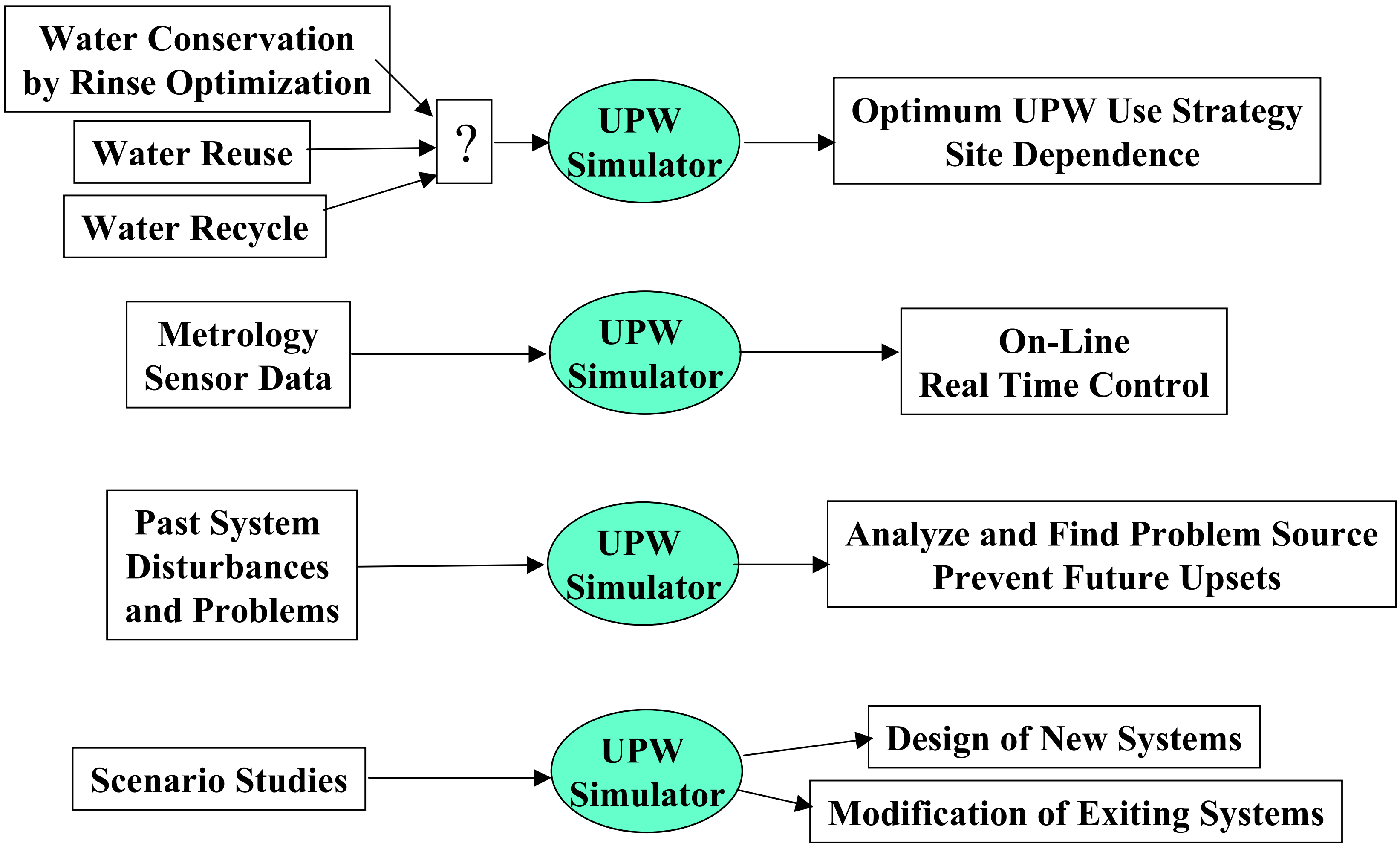
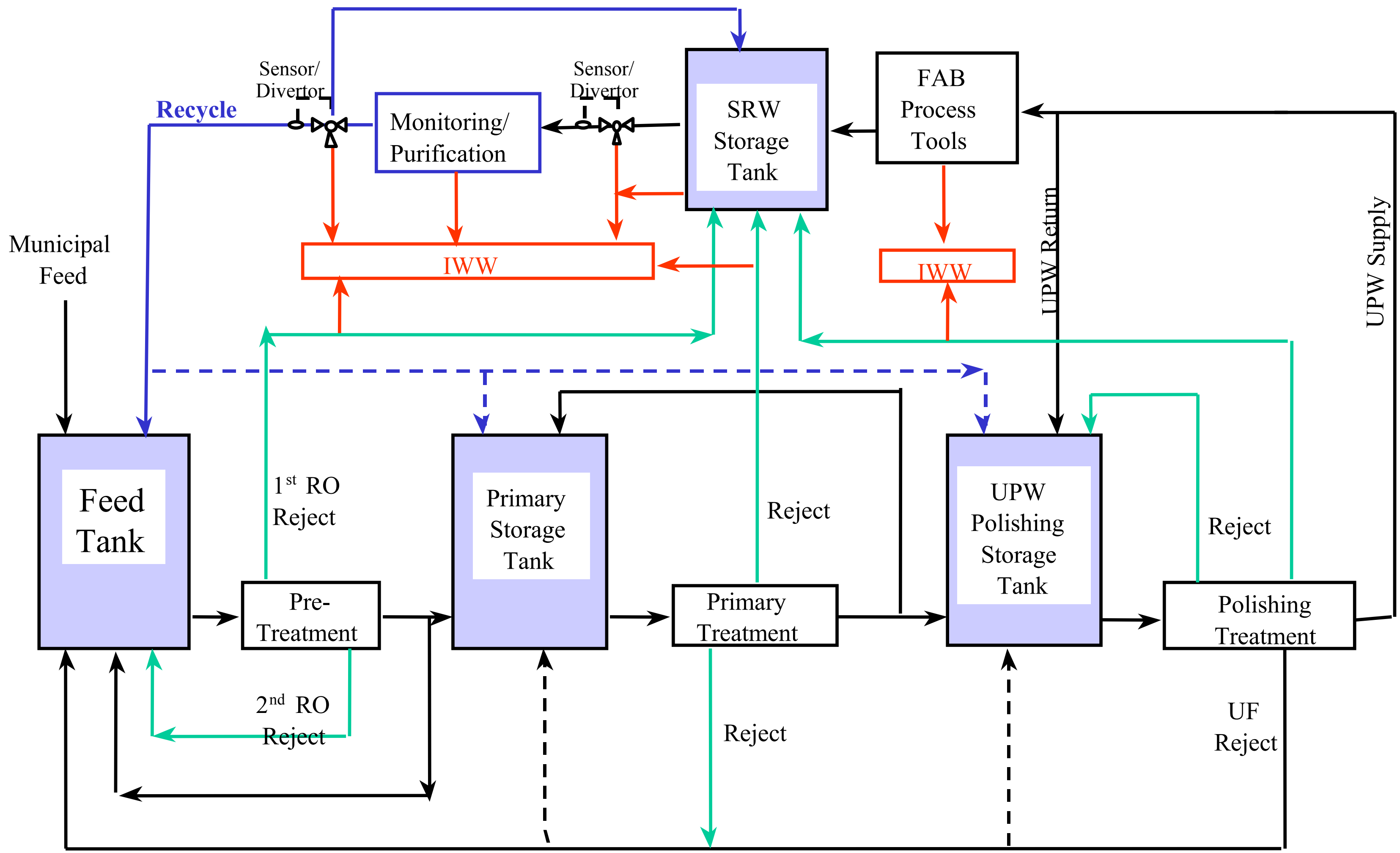
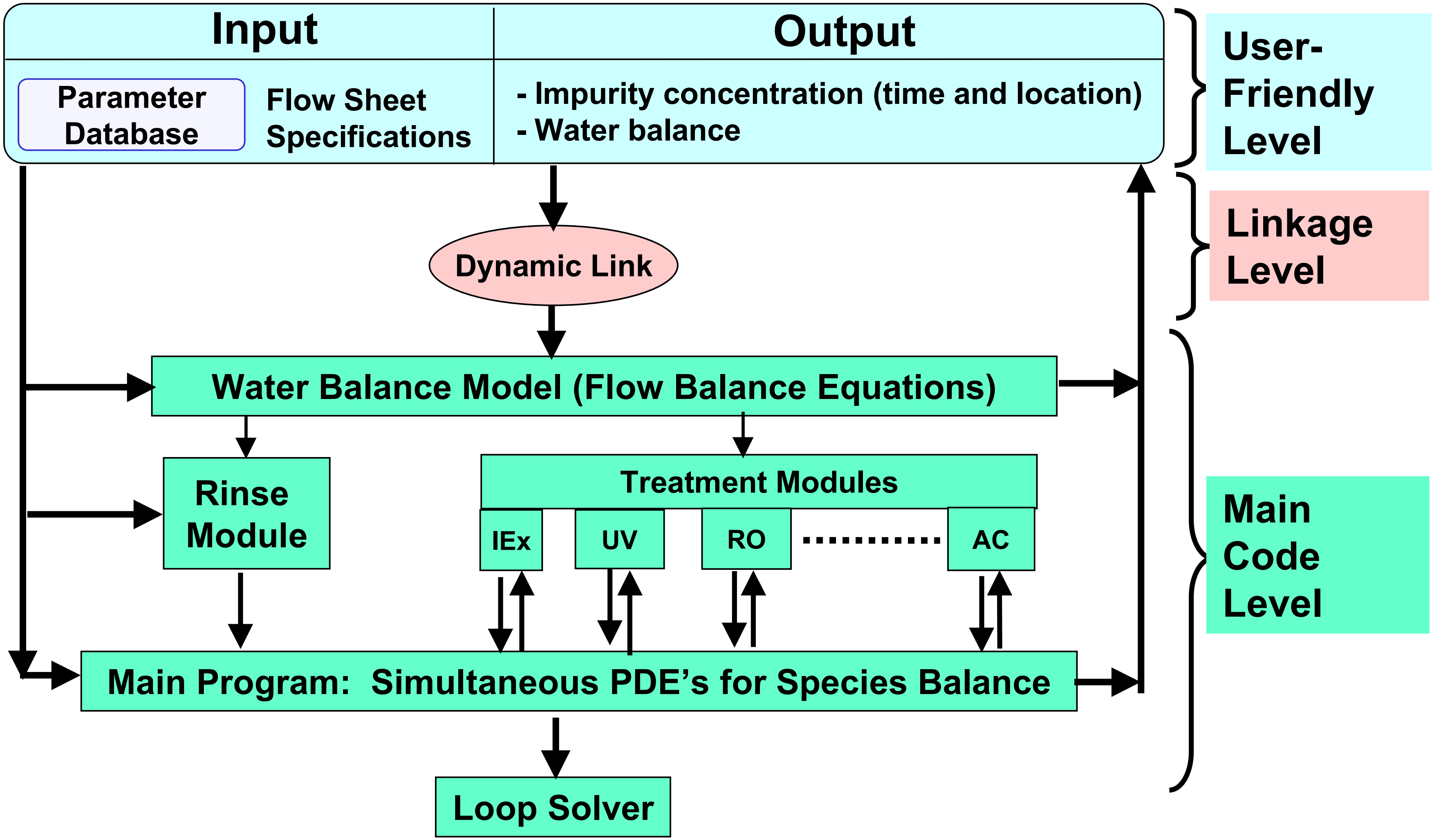
Significance and Application of UPW Simulator



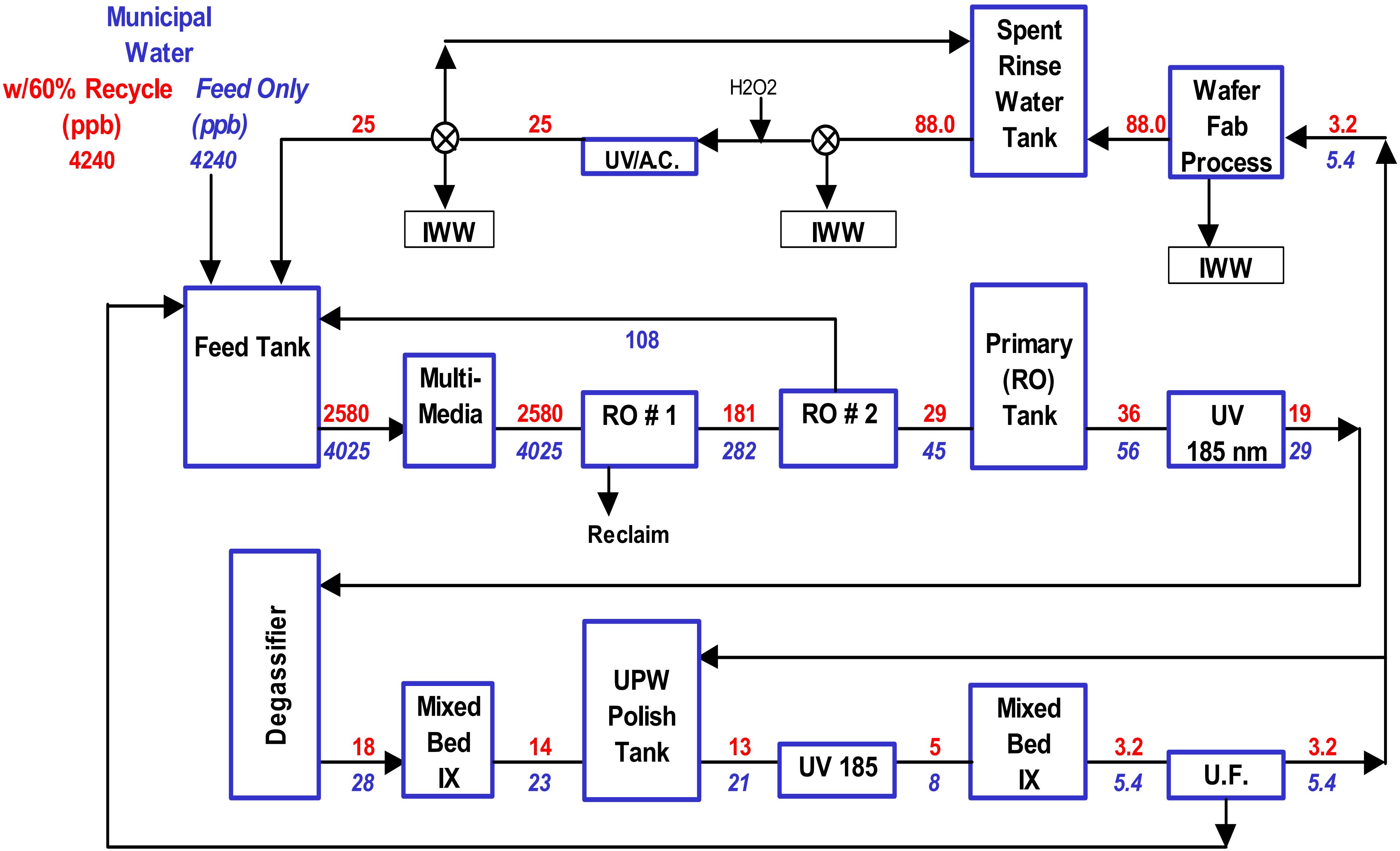
UPW System with Recycle Options



Structure of the UPW Recycle Simulator



UPW Simulation: TOC Concentrations



Multi-component Model for Adsorption Processes

Activated Carbon/Ion Exchange - Three Phase Model

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:

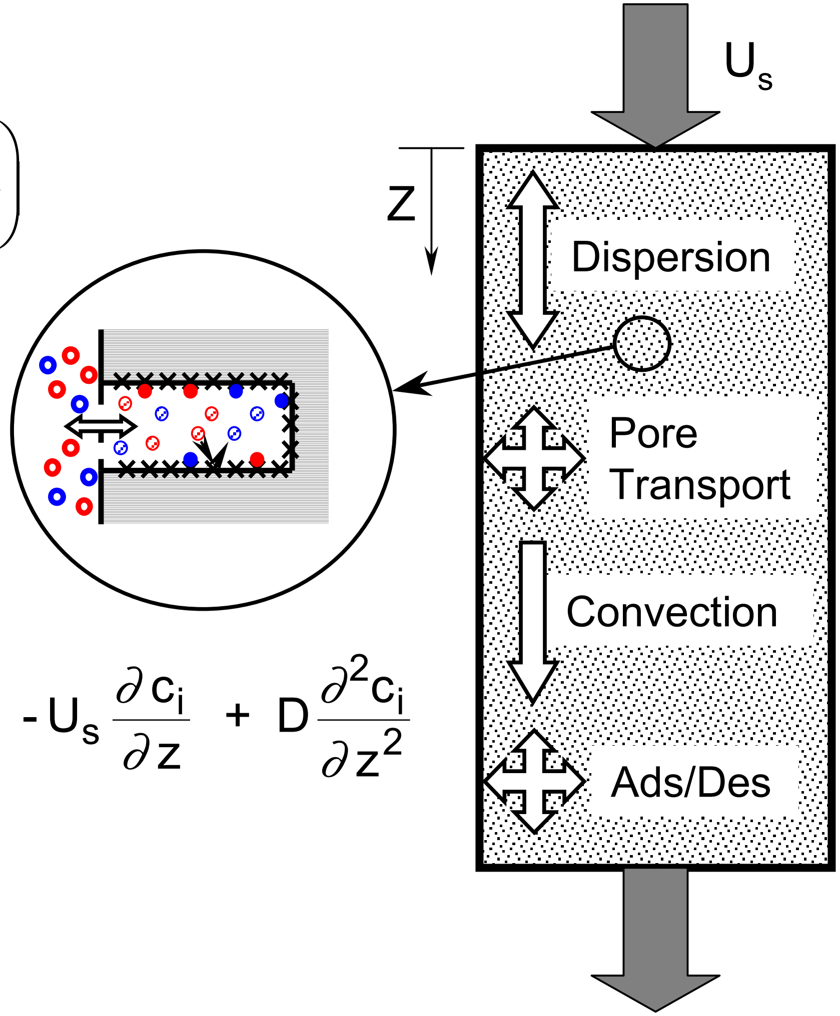
$$\varepsilon_p \frac{\partial p_i}{\partial t} + \frac{\partial s_i}{\partial t} = \alpha\, k_{pi} (c_i - p_i)$$

Bulk Fluid Phase Conservation:

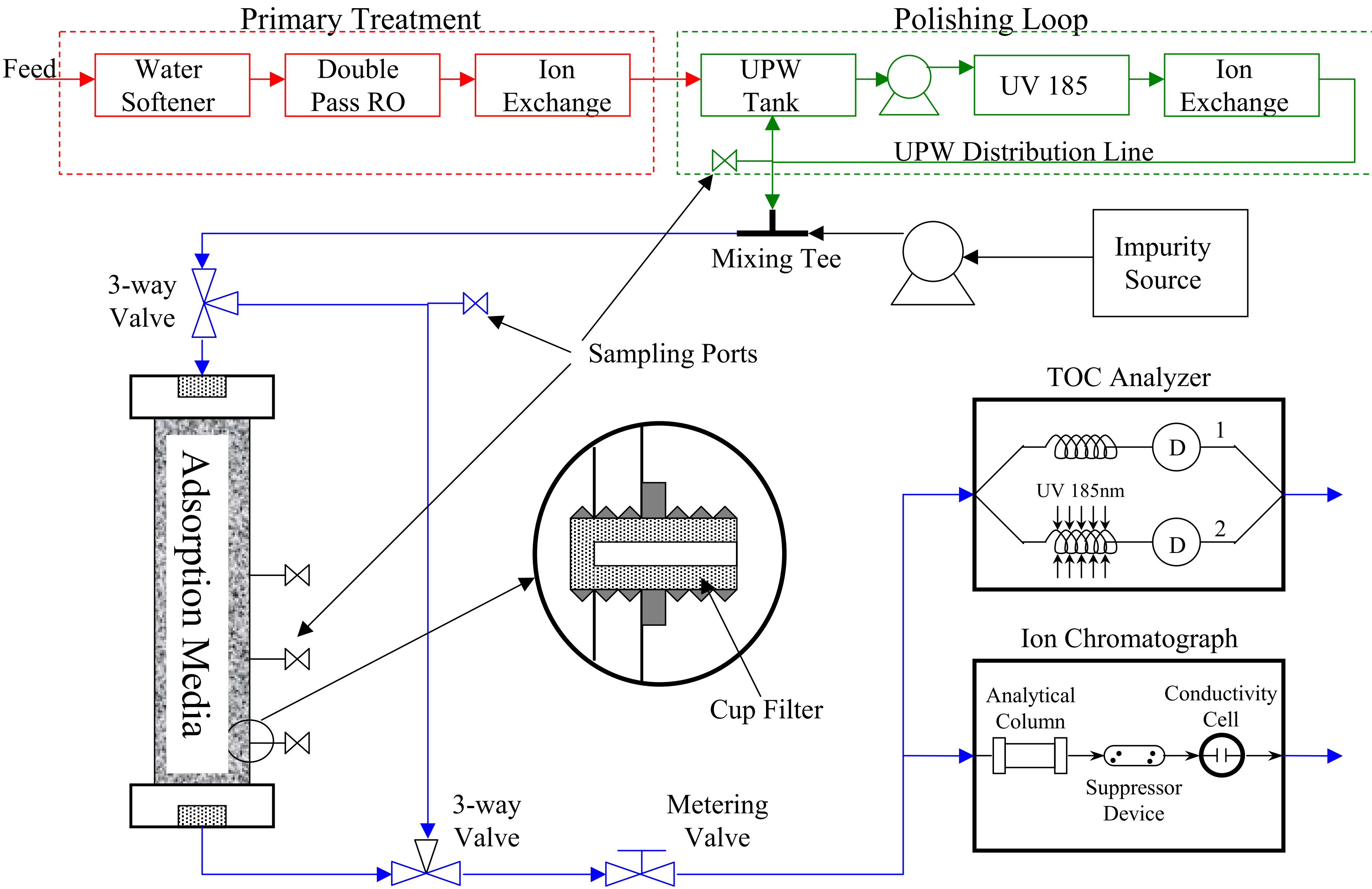
$$\varepsilon_b \frac{\partial c_i}{\partial t} + \varepsilon_p (1 - \varepsilon_b) \frac{\partial p_i}{\partial t} + (1 - \varepsilon_b) \frac{\partial s_i}{\partial t} = - U_s \frac{\partial c_i}{\partial z} + D \frac{\partial^2 c_i}{\partial z^2}$$

Sites Conservation:

$$s_o = s + \sum_i s_i$$

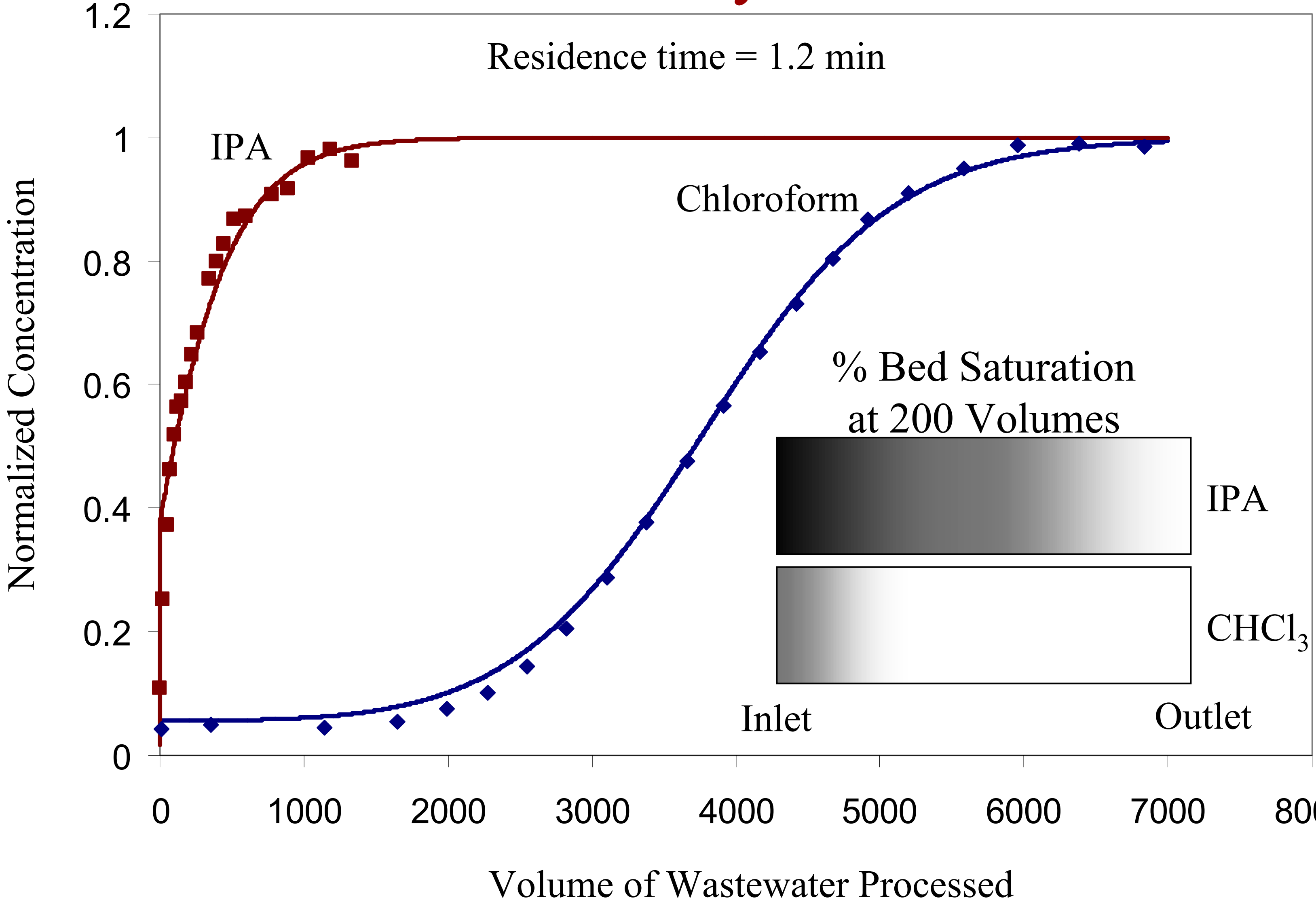


Study of Interactions Involving Adsorption Treatment

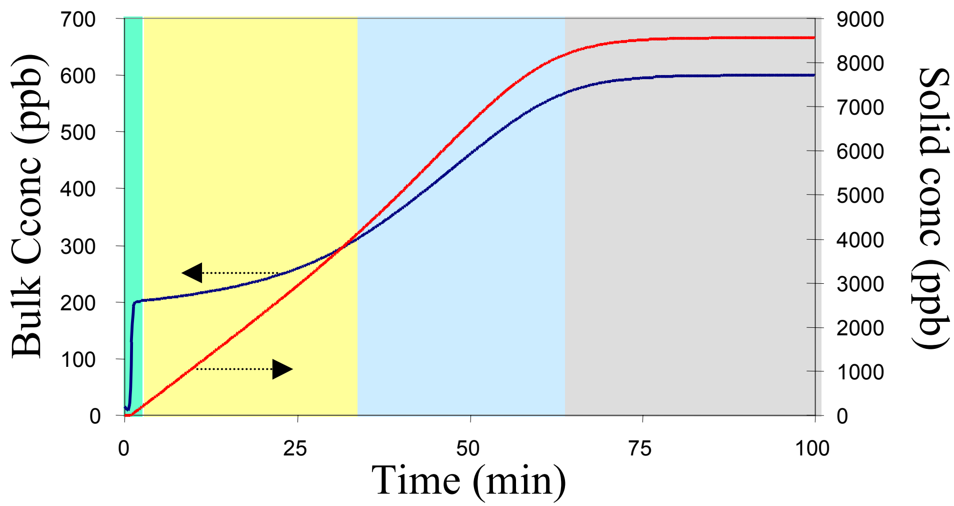


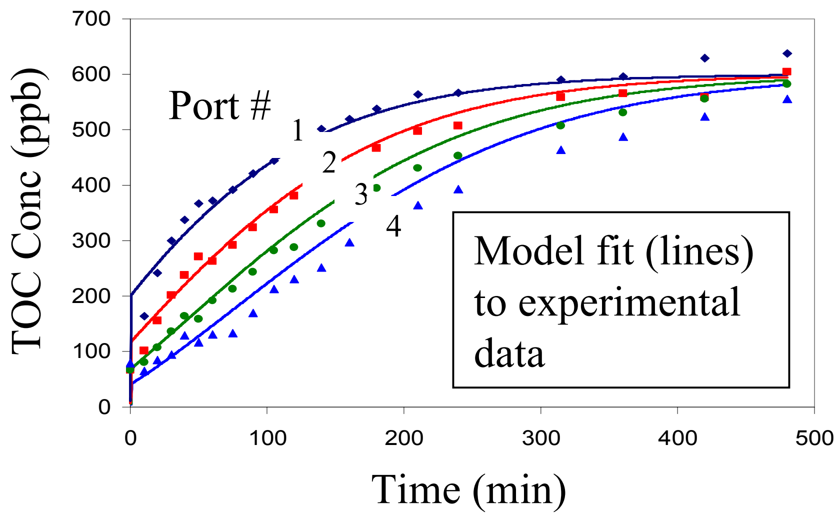
NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing

Compound Dependence of Purification in Activated Carbon Systems



TOC Adsorption on Granulated Activated Carbon





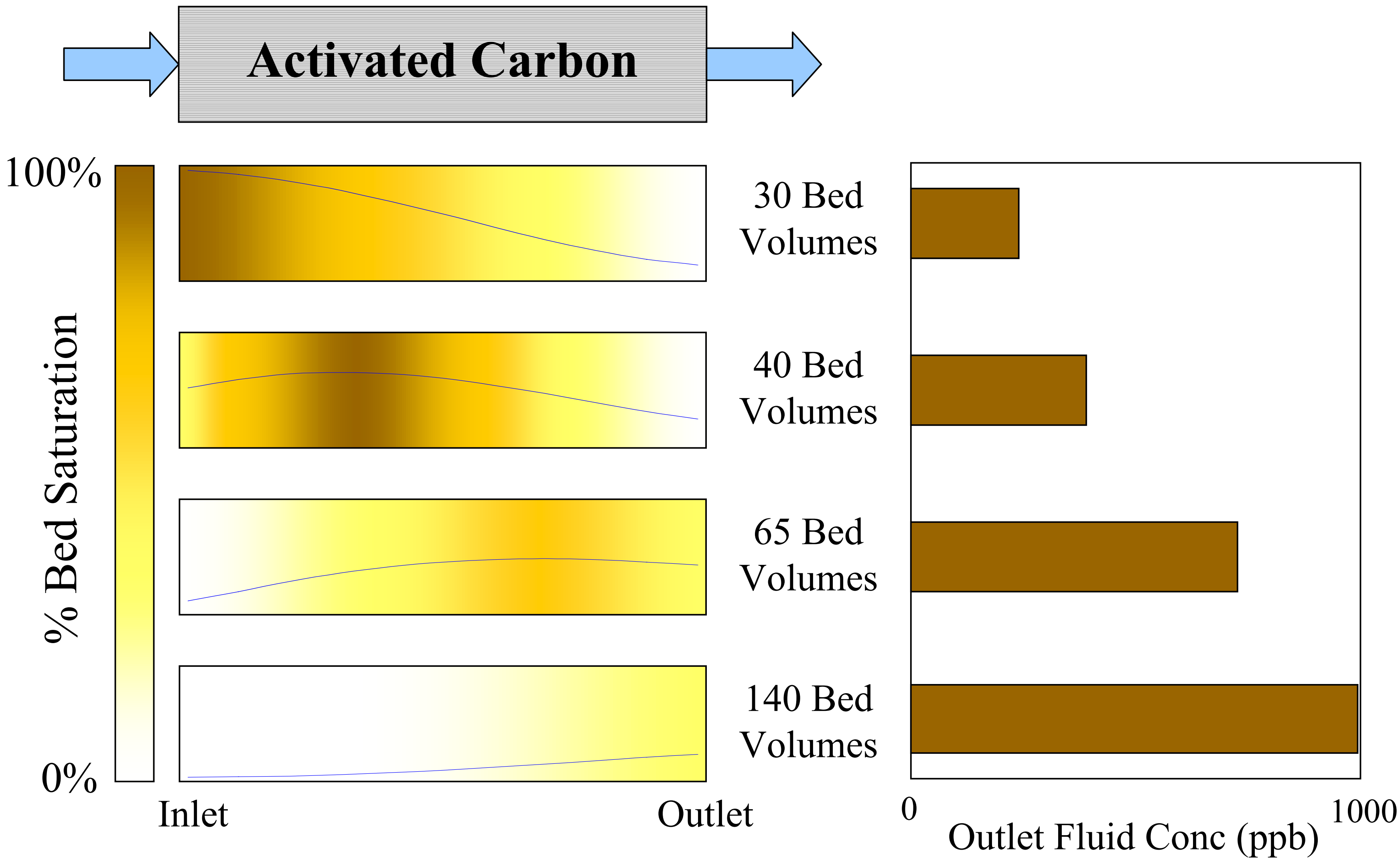
Initial wash out period. Bulk flow characteristics and mass transfer effects dominate.

Fresh adsorbent in some parts of packed bed.

Partially deactivated adsorbent in all parts of packed bed.

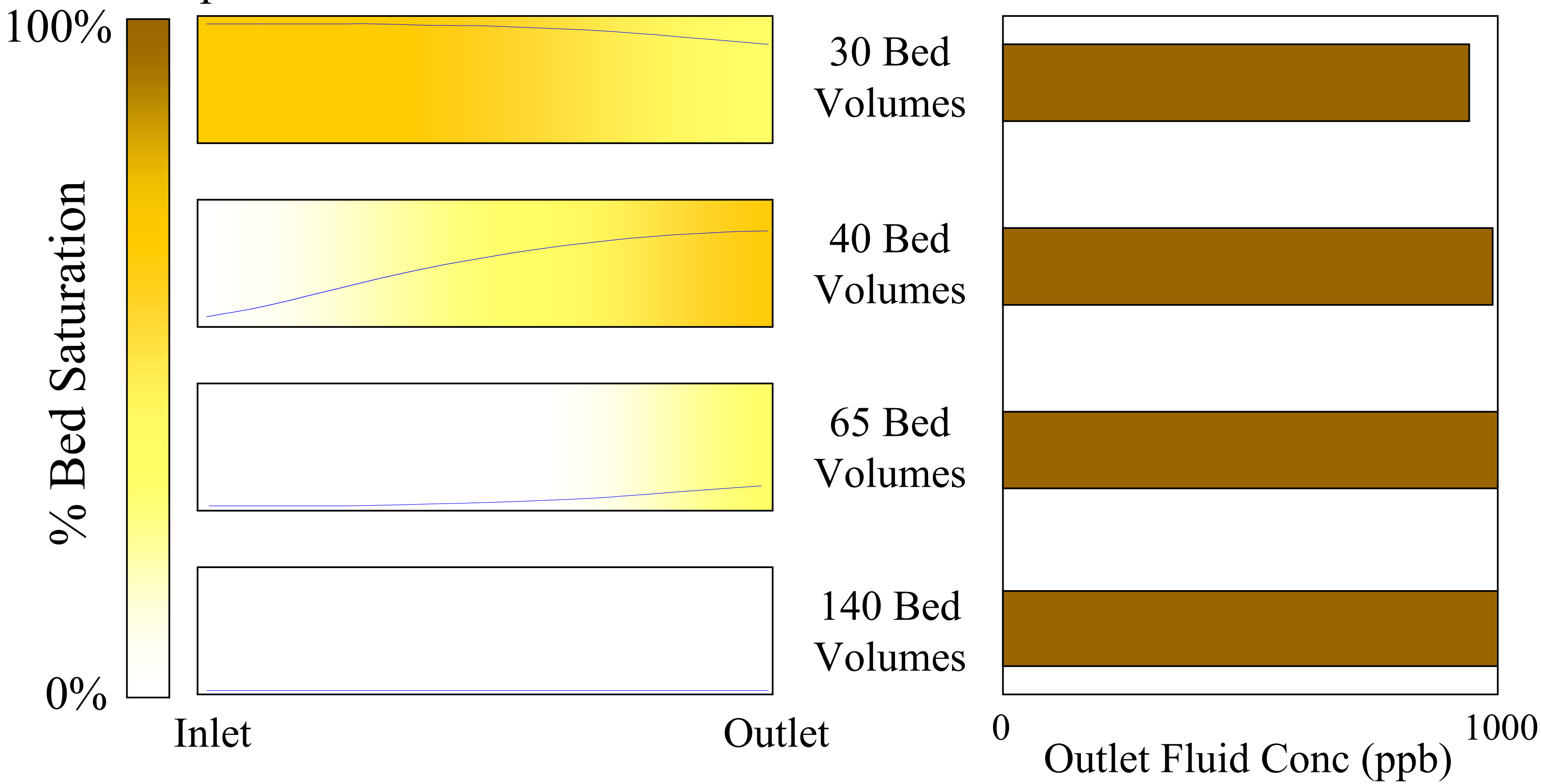
Total bed exhaustion.

Movement of Ethylene Glycol in Solid Phase During Purge



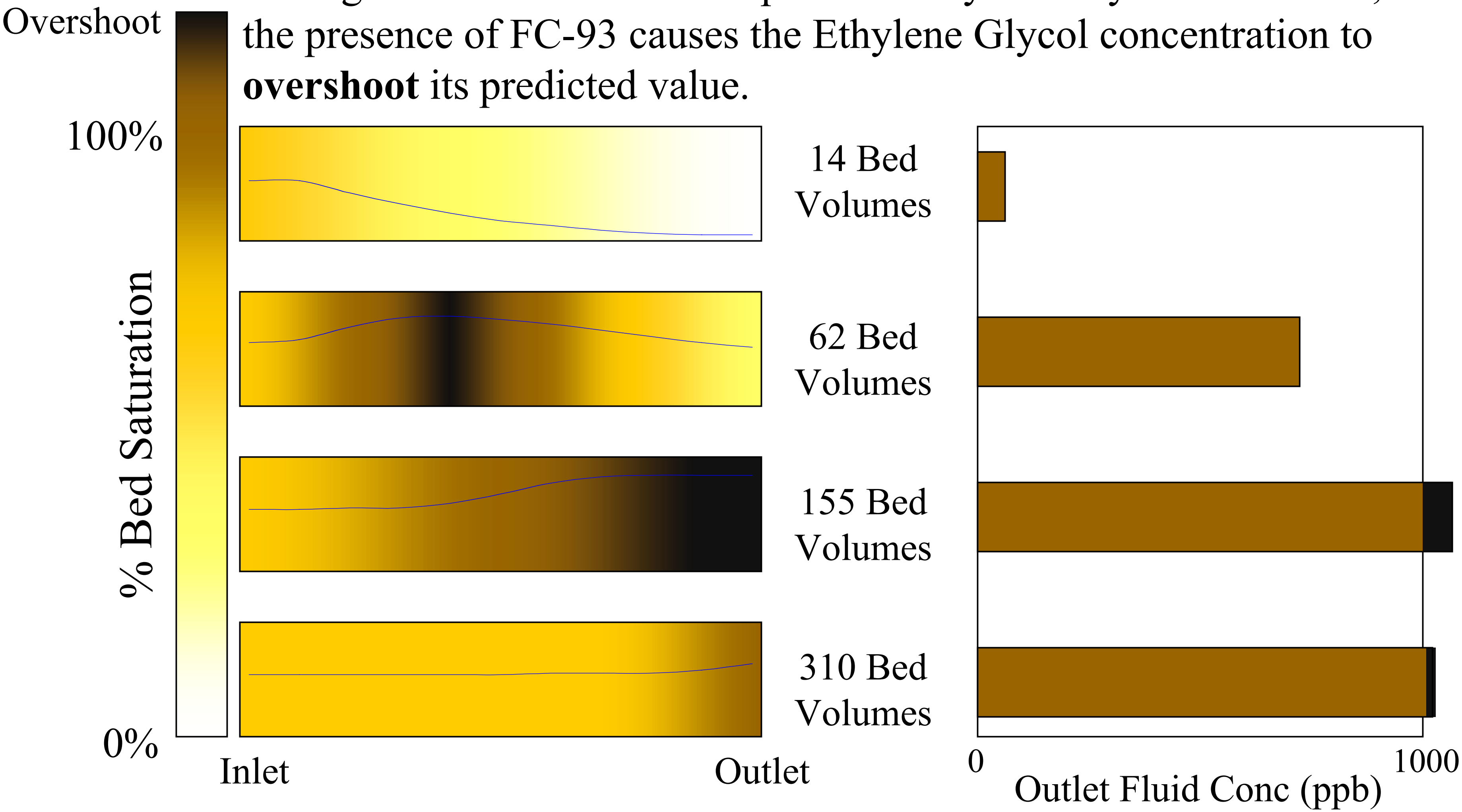
Multi-Component Interaction - Type I: Alteration of Kinetic Behavior

The presence of HCl during the purging of Ethylene Glycol causes the Ethylene Glycol concentration front to **move more quickly** through the packed bed.

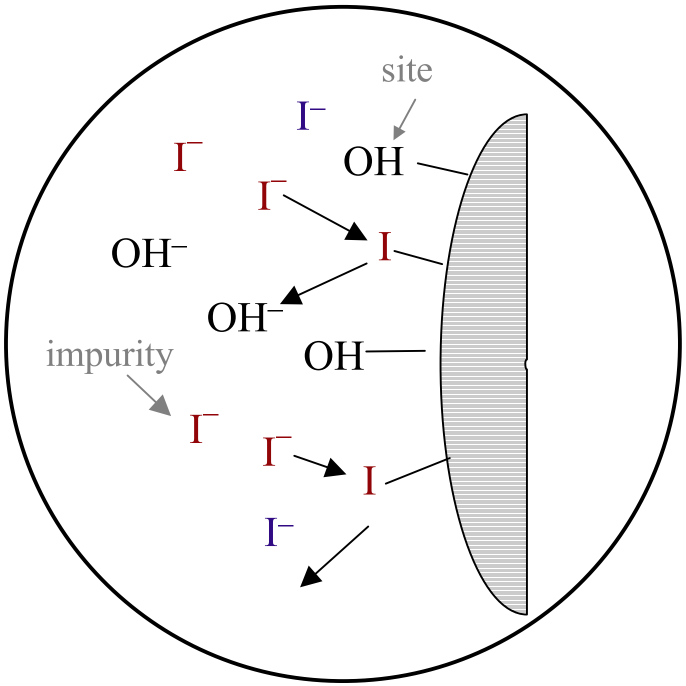


Multi-Component Interaction - Type II: Competitive Adsorption

During the simultaneous adsorption of Ethylene Glycol and FC-93, the presence of FC-93 causes the Ethylene Glycol concentration to **overshoot** its predicted value.



Enhanced Ion Exchange for Treatment of Rinse Wastewater



Anion Exchange Reaction:

$$I_i^{-\nu_i} + \nu_i R\text{-}OH \underset{k_{di}}{\overset{k_{ai}}{\leftrightarrow}} \nu_i OH^- + R_{\nu_i} I_i$$

Cation Exchange Reaction:

$$I_i^{+\nu_i} + \nu_i R\text{-}H \underset{k_{di}}{\overset{k_{ai}}{\leftrightarrow}} \nu_i H^+ + R_{\nu_i} I_i$$

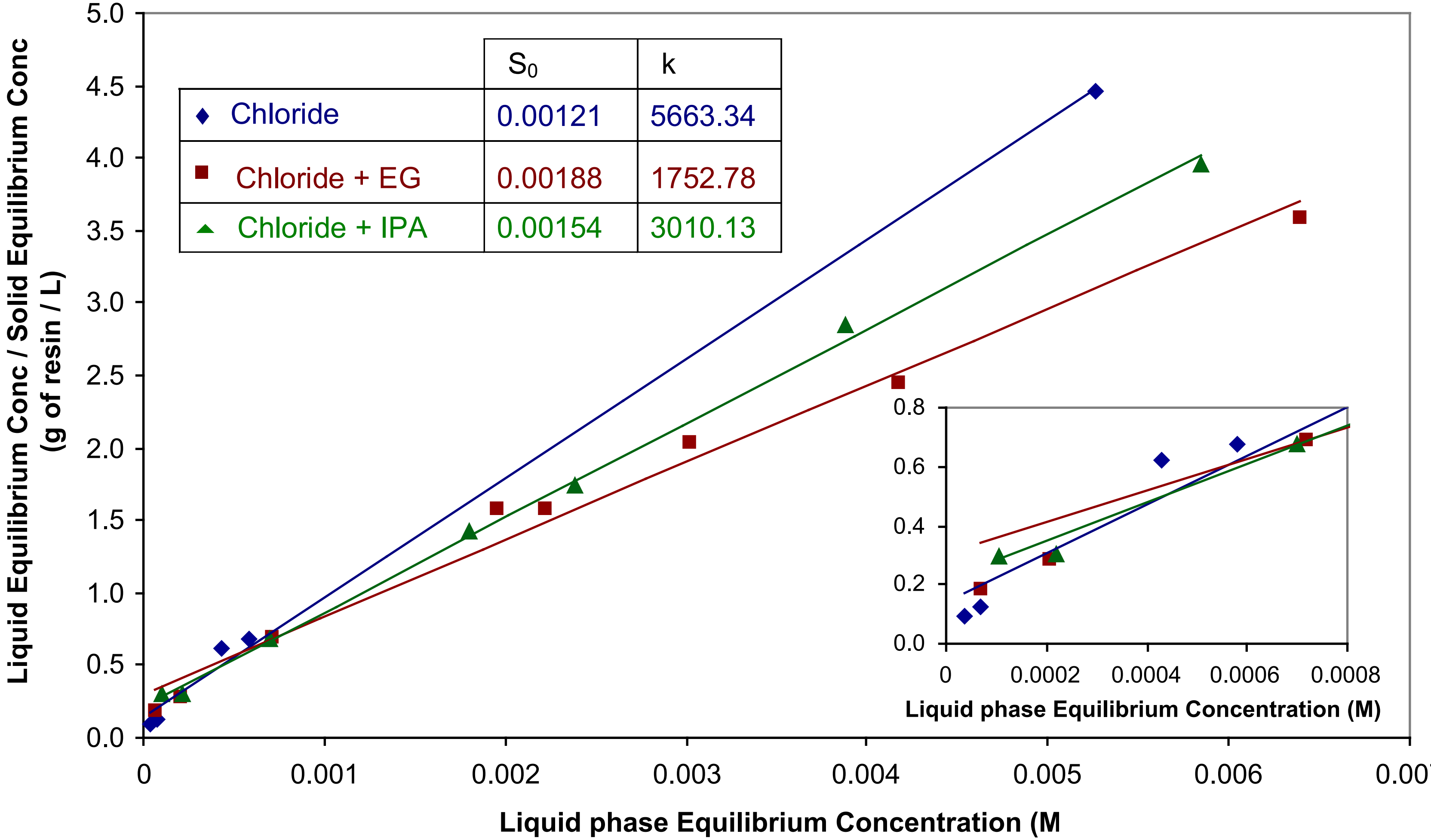
Langmuir Isotherm:

$$S_I = \frac{k\, C_I}{1 + k\, C_I} S_0$$

S_I - Solid phase equilibrium concentration

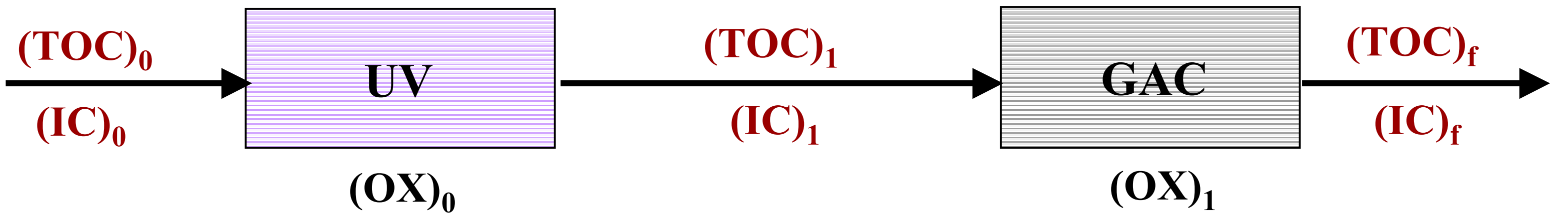
C_I - Liquid phase equilibrium concentration

Enhancement of Ion Exchange Performance in Wastewater Treatment



	S_0	k
Chloride	0.00121	5663.34
Chloride + EG	0.00188	1752.78
Chloride + IPA	0.00154	3010.13

A Novel Method Utilizing UV and GAC Interactions for Treatments of Rinse Wastewater



$$(H_2O, H_2O_2, O_3) + h\nu \rightarrow (OX)_0$$

$$(TOC)_0 + (OX)_0 \rightarrow (IC)_1$$

$$(TOC)_0 + h\nu \rightarrow (TOC)_1$$

$$(TOC)_1 + (OX)_0 \rightarrow (TOC)_1$$

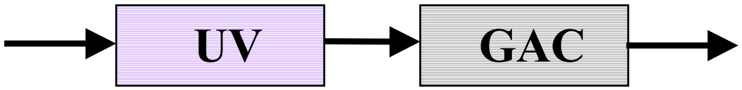
- Effective use of waste water ingredients (eg. H_2O_2)
- Takes advantage of both partial and total oxidation

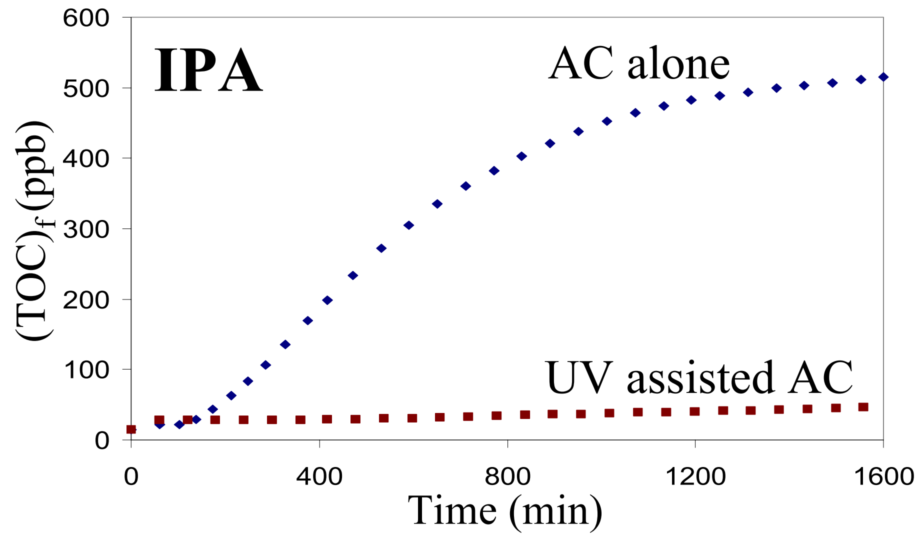
$$(TOC)_1 + GAC \rightarrow (TOC)_a$$

$$(TOC)_a + (OX)_1 \rightarrow (IC)_f$$

- Regenerative Adsorption
- More efficient oxidation due to:
  - Capture of TOC
  - Concentration of TOC

UV-Assisted TOC Removal by Activated Carbon



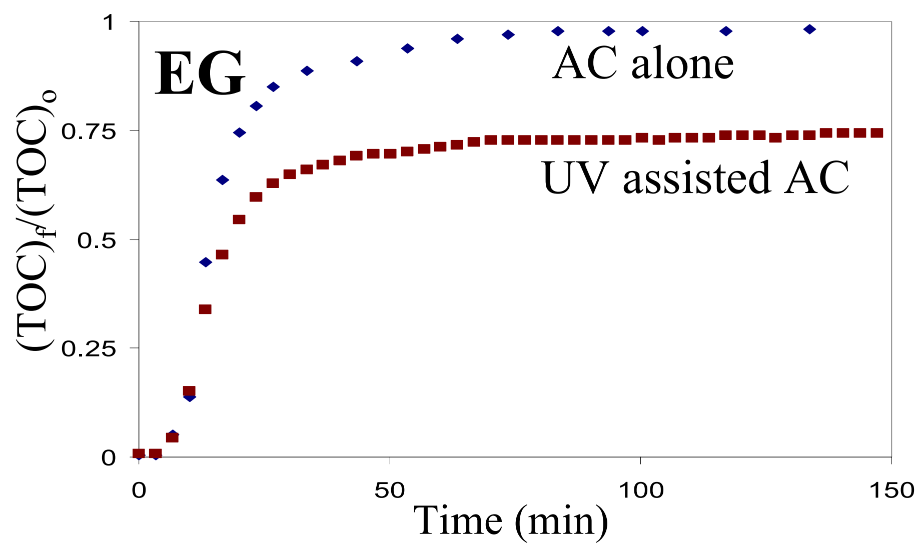


I: Hard to remove organics by total oxidation or by AC

II: Partially reacted organics; enhanced attraction to and retention by the carbon bed;

III: Converts the activated-carbon bed to a high-capacity absorber, self cleaning reactor

**** If designed properly, the techniques will take advantage of residual H_2O_2 in the rinse water.**



Conclusions

- Proper Utilization of Simulation Techniques Leads to:
  - Optimization of water conservation/reuse/recycle
  - Design of novel purification techniques and systems
  - Design of new systems
  - Optimization of existing systems
- Analytical Simulation of Unit Processes Leads to:
  - Fundamental understanding of process dynamics
  - Evaluation of hard-to-measure parameters
- Future Application Will Include:
  - Prevention of system upsets
  - On-line and real-time process control