Modeling and Simulation of Multicomponent Adsorption of Organic Acids from Aqueous Solutions

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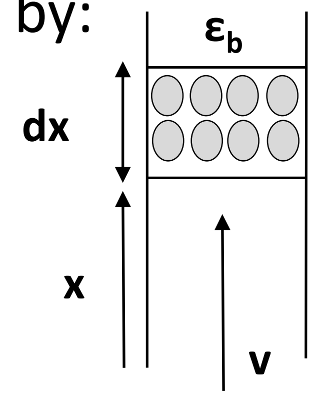
Governing equations for a fixed-bed adsorber

- Differential mass balance for adsorption of c (z,t) is given by:



Accumulation rate of C =rate of C {[in by dispersion]-[out by dispersion]
+[in by convection]-[out by convection]-[loss by adsorption]}

Liquid phase

1

$$-D_L\frac{\partial^2 c}{\partial x^2}+\frac{\partial vc}{\partial x}+\frac{\partial c}{\partial t}+\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{3}{r_p}k_f\left(c-c_{p,r=rp}\right)=0$$

Solid phase

2

$$\varepsilon_p\frac{\partial c_p}{\partial t}+\rho_p\frac{\partial q_p}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\varepsilon_p D_p\frac{\partial c_p}{\partial r}\right)\right]$$

3

$$q_p=\frac{q_m k c_p}{1+kc_p}$$

Initial and boundary conditions

$$0<x<L, t=0:\ c=0$$

$$x=0, t>0: D_L\frac{\partial^2 c}{\partial x^2}=v(c_{x=0}-c_0)$$

$$x=L, t>0: \frac{\partial c}{\partial x}_{x=L}=0$$

$$0<r<r_p, t=0:\ c_p=0, q_p=0$$

$$r=0, t>0:\ \frac{\partial c_p}{\partial r}_{r=0}=\frac{\partial q_p}{\partial r}_{r=0}=0;\ r=r_p, t>0:\ \varepsilon_p D_p\frac{\partial c_p}{\partial r}_{r=r_p}=k_f\left(c-c_{p,r=rp}\right)$$

Governing equations for a fixed-bed adsorber

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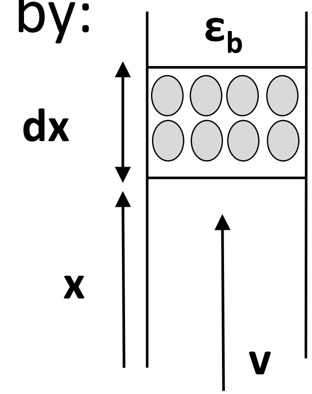

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$$\varepsilon_p \frac{\partial c_p}{\partial t} + \rho_p \frac{\partial q_p}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\varepsilon_p D_p \frac{\partial c_p}{\partial r}\right)\right]$$

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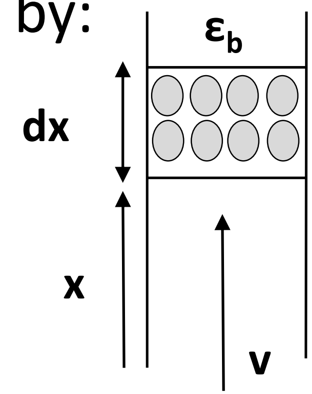

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Outline

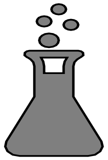
- Overview of bioconversion processes to produce organic acids from biomass and biomass wastes
- Downstream separation processes for extraction of organic acids from fermentation broths at low pH
- Adsorption equilibrium and kinetics in the sorption of organic acids
- Fixed-bed sorption dynamics and adsorber configurations for enhanced recovery
- Multicomponent adsorption dynamics

Introduction

Biobased or chemical based?

Organic acids

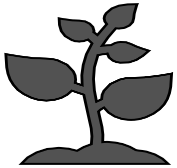
Chemical process



Petroleum, natural gas

Low cost but unsustainable

Biobased production

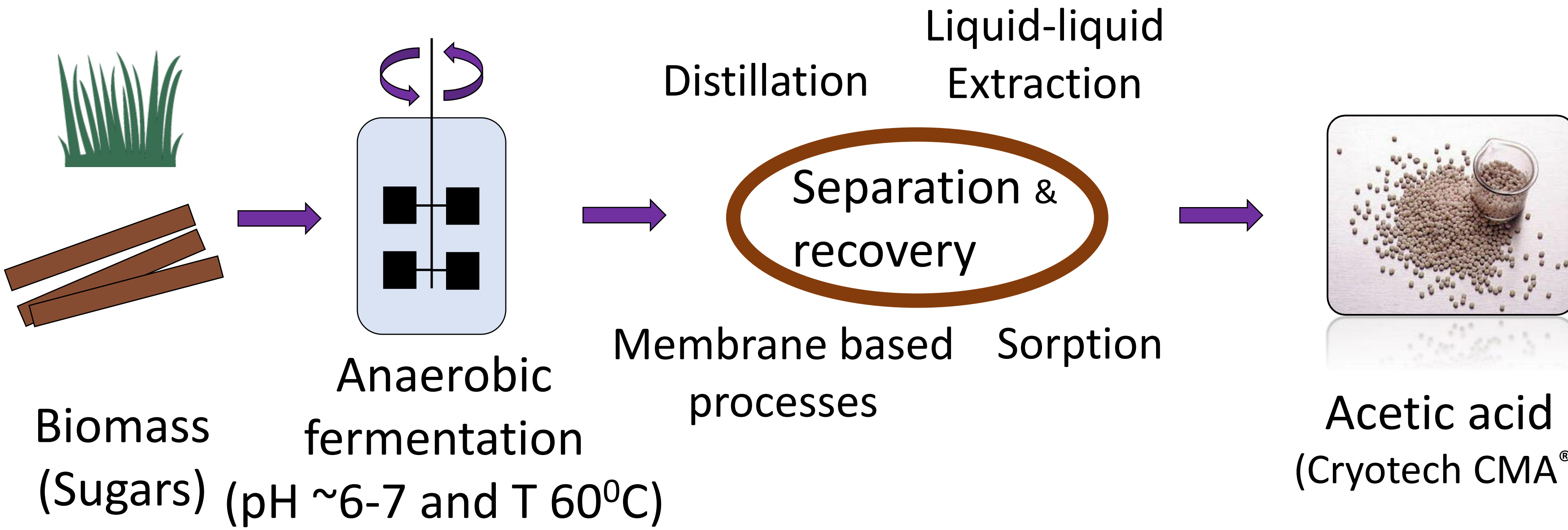


Organic waste materials

Sustainable and renewable

- Global acetic acid demand ~ 13 million tons in 2015[1]
- 65% of acetic acid produced via methanol carbonylation[2]
- Global lactic acid demand expected to reach 1.9 million tons by 2020[3]
- >90% of lactic acid produced via fermentation[3]
- By 2100, more than 95% of chemicals and polymers are envisioned to be produced from renewable resources[4]

Production of organic acids from renewable sources and the need for efficient recovery



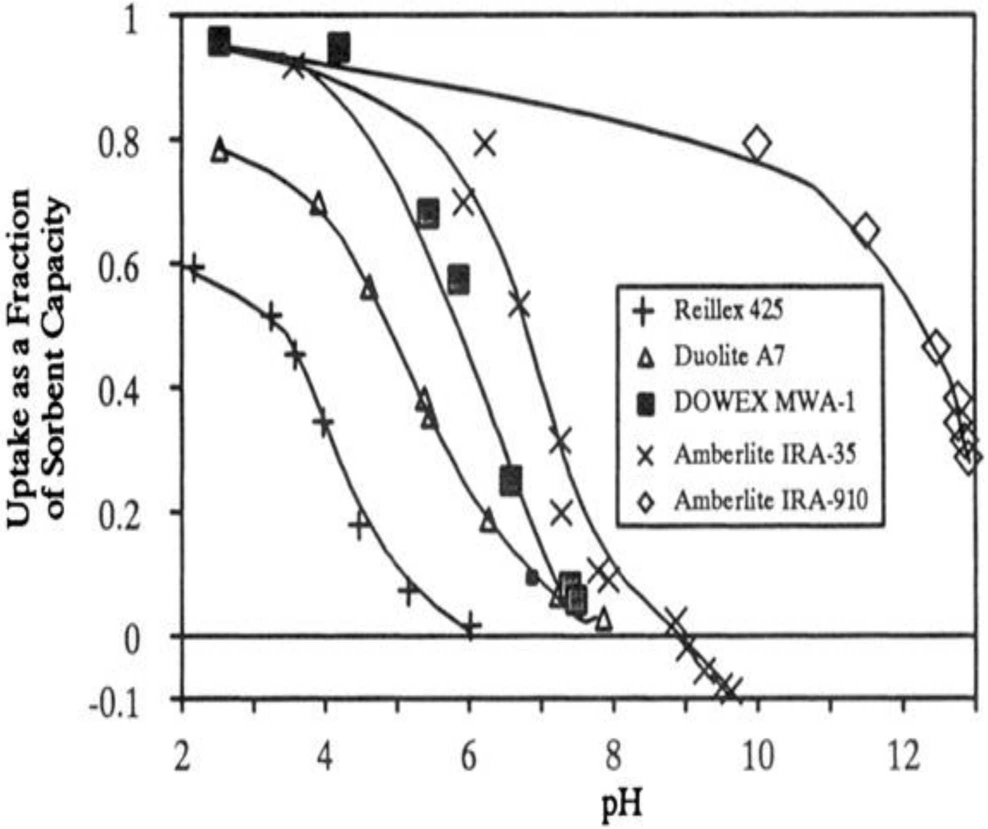
- Acetic acid uses in food, polymer, and other industries. Emerging use in production of calcium magnesium acetate (CMA) road deicer and potassium acetate (KA) aircraft deicer
- CMA from synthetic acetic acid ~$1900 per ton
- CMA is biodegradable and an environmentally benign alternative for rock salt with a potential demand of 25 million tons per year in North America[3]

Anaerobic fermentation of carbohydrates to acetic acid

Bacteria	pH	T
• *Clostridium thermoaceticum*	6.5 – 7.0	~ 60°C
• *C. thermoaceticum* and *M. thermoautotrophica*	6.4 – 7.0	~ 60°C
• *C. formicoaceticum* and *L. lactis*	7.6	~ 58°C

Adsorption for recovery of acetic and lactic acids from aqueous solutions

Tung and King, 1994

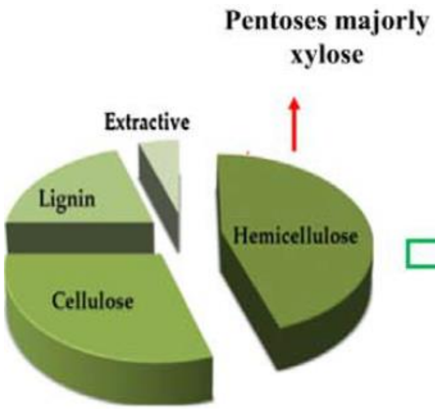


- Uptake capacity of weak base resins decrease with increase in solution pH
- Not feasible to economically recover acetic or lactic aid at neutral pH

Challenges in the application of bioprocesses for acetic acid production:

- ➢ Conduct fermentation at low pH and ambient temperature
- ➢ Enhance bed capacity utilization

Novel low pH fermentation process for the production of organic acids from biomass and biomass wastes

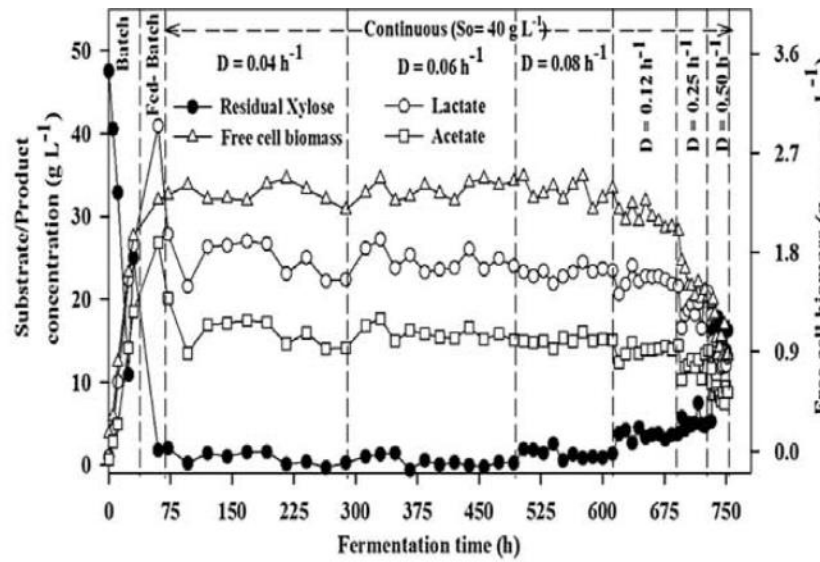


Typical composition of biomass and biofiber

Xylose

L. buchneri immobilized in alumina fibers in CSTR

Anoxic fermentation
(pH ~4 and T 35^0C)



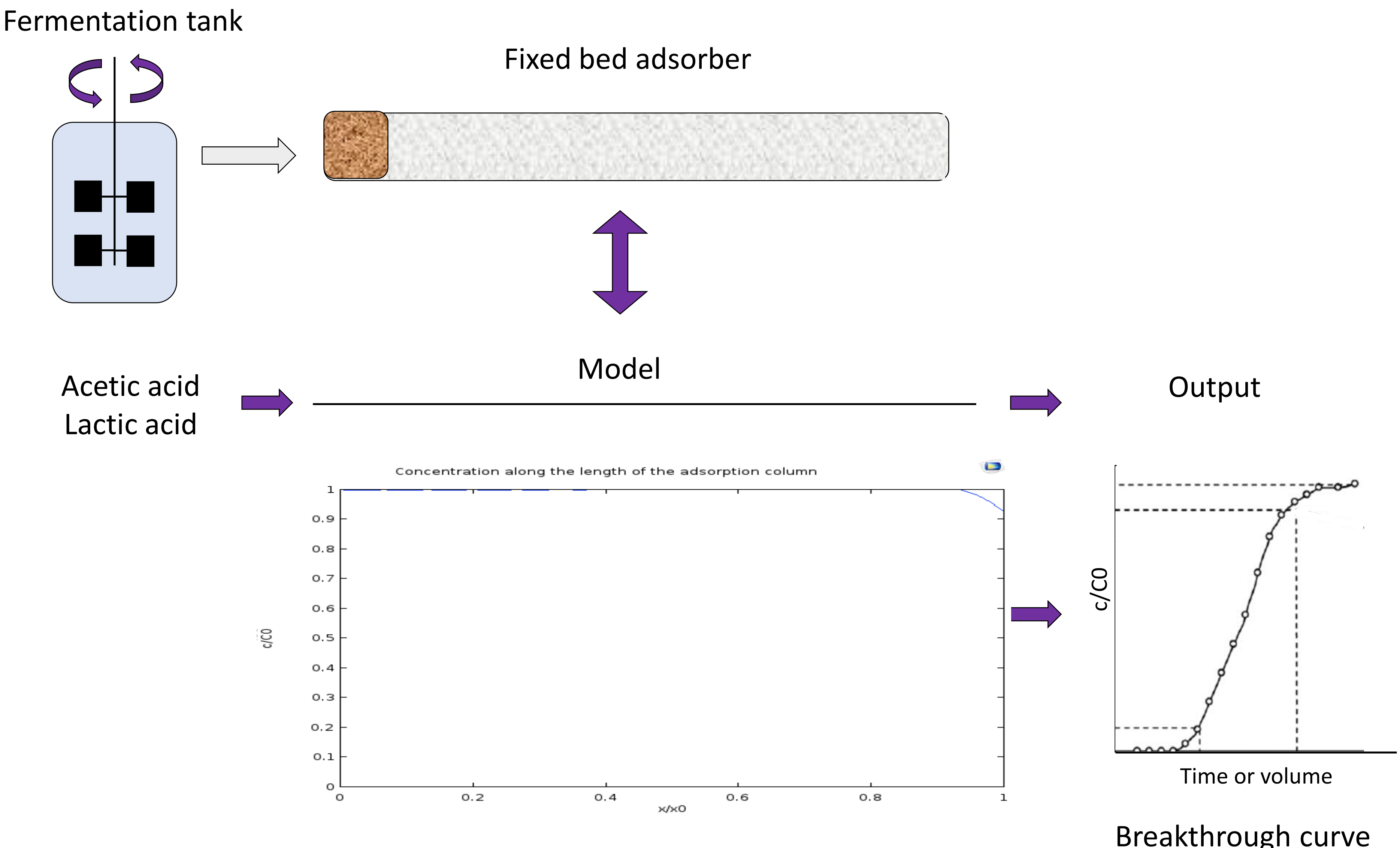
Veeravalli and Mathews, 2018

- Novel pH ~4 bacterial fermentation for acetic and lactic acids production using xylose
- 32 g/L acetic acid and 67 g/L lactic acid were produced in fed batch fermentation

Objectives

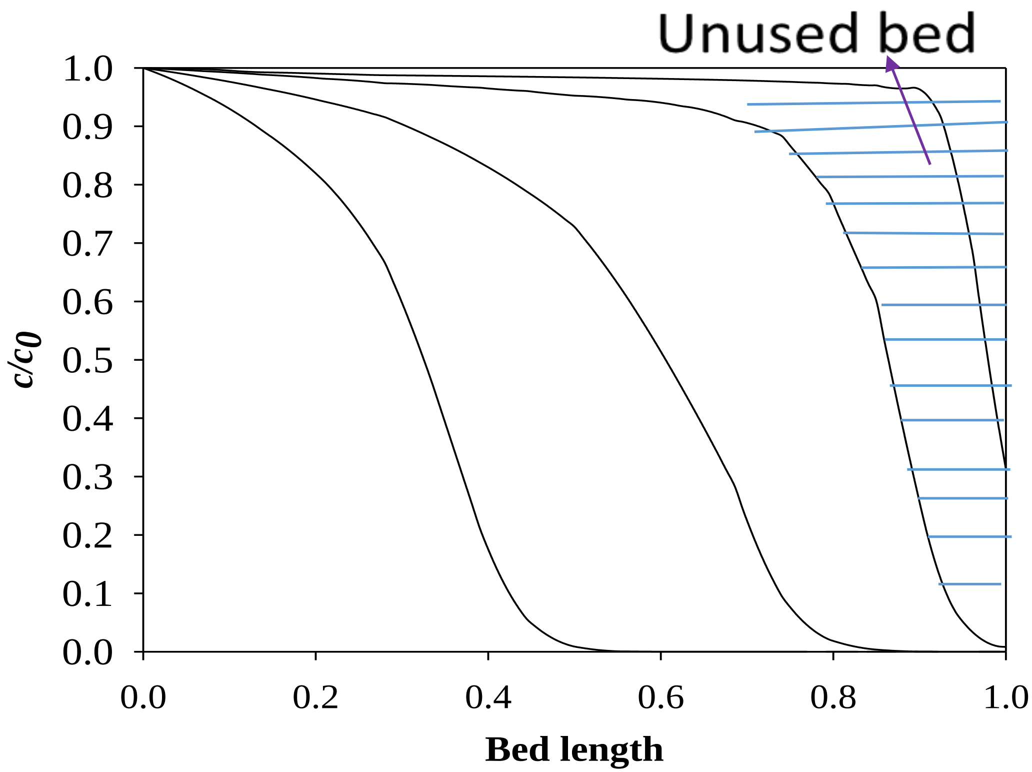
- Recovery of acetic and lactic acids at low pH using adsorption technology
- Evaluation of adsorption contactor for enhanced bed capacity utilization
- Modeling of sorption process on granular activated carbon (GAC) and synthetic resins
- Implementation of model solution using COMSOL software

Fixed-bed adsorbers to recover organic acids from fermentation broth

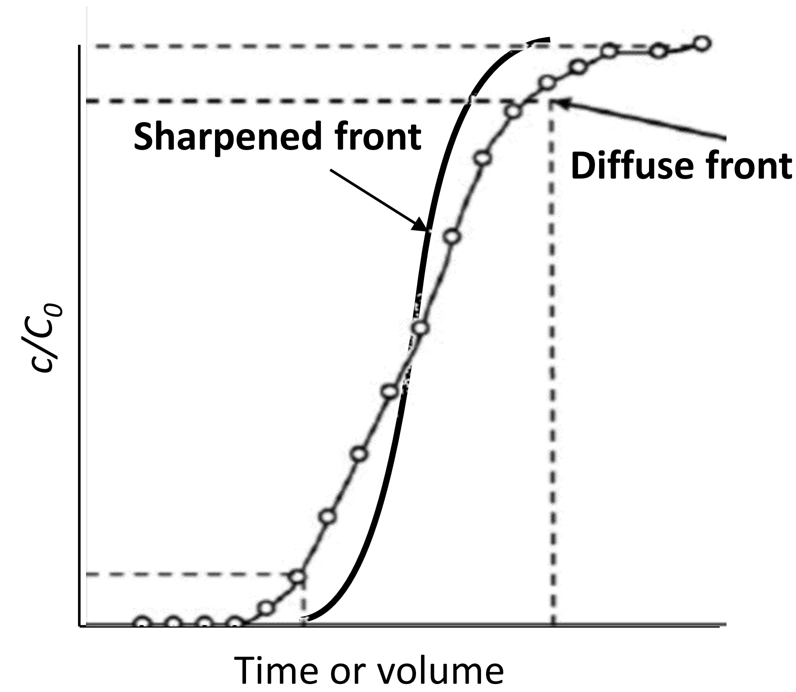


Bed capacity utilization

Concentration profile along the bed length

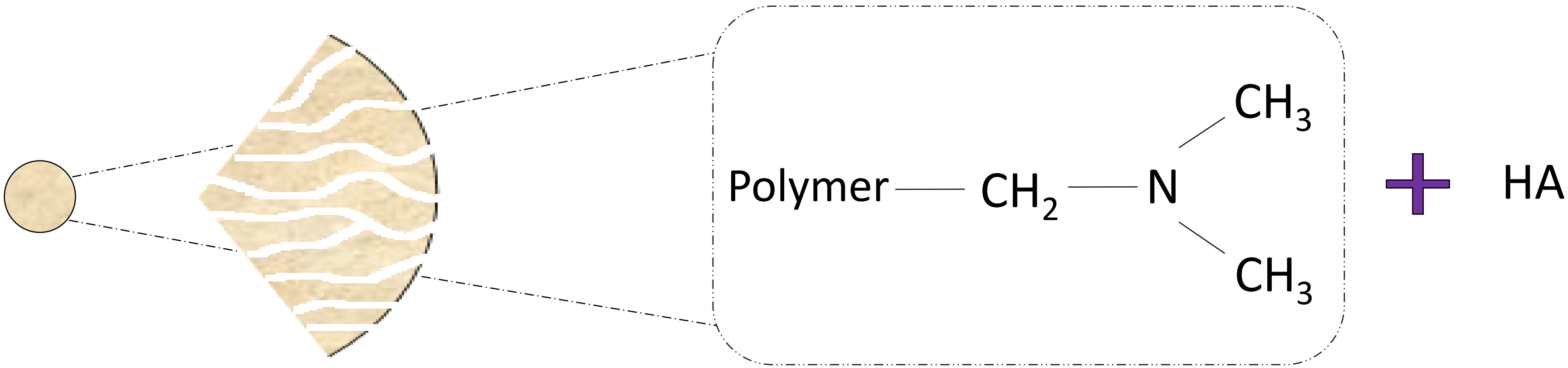


Breakthrough curve

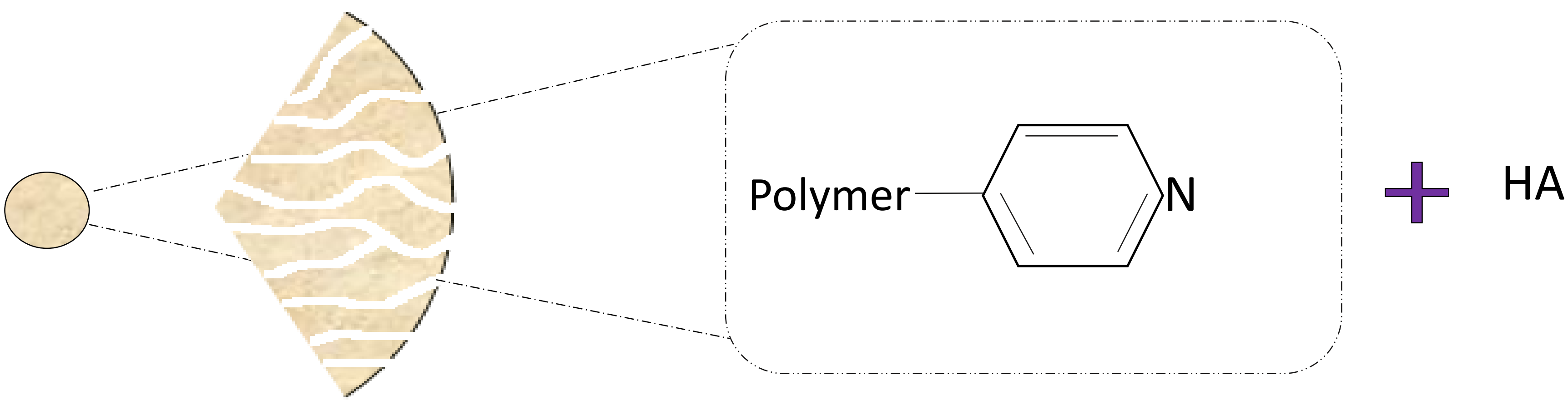


Adsorption of organic acids on weak base resins

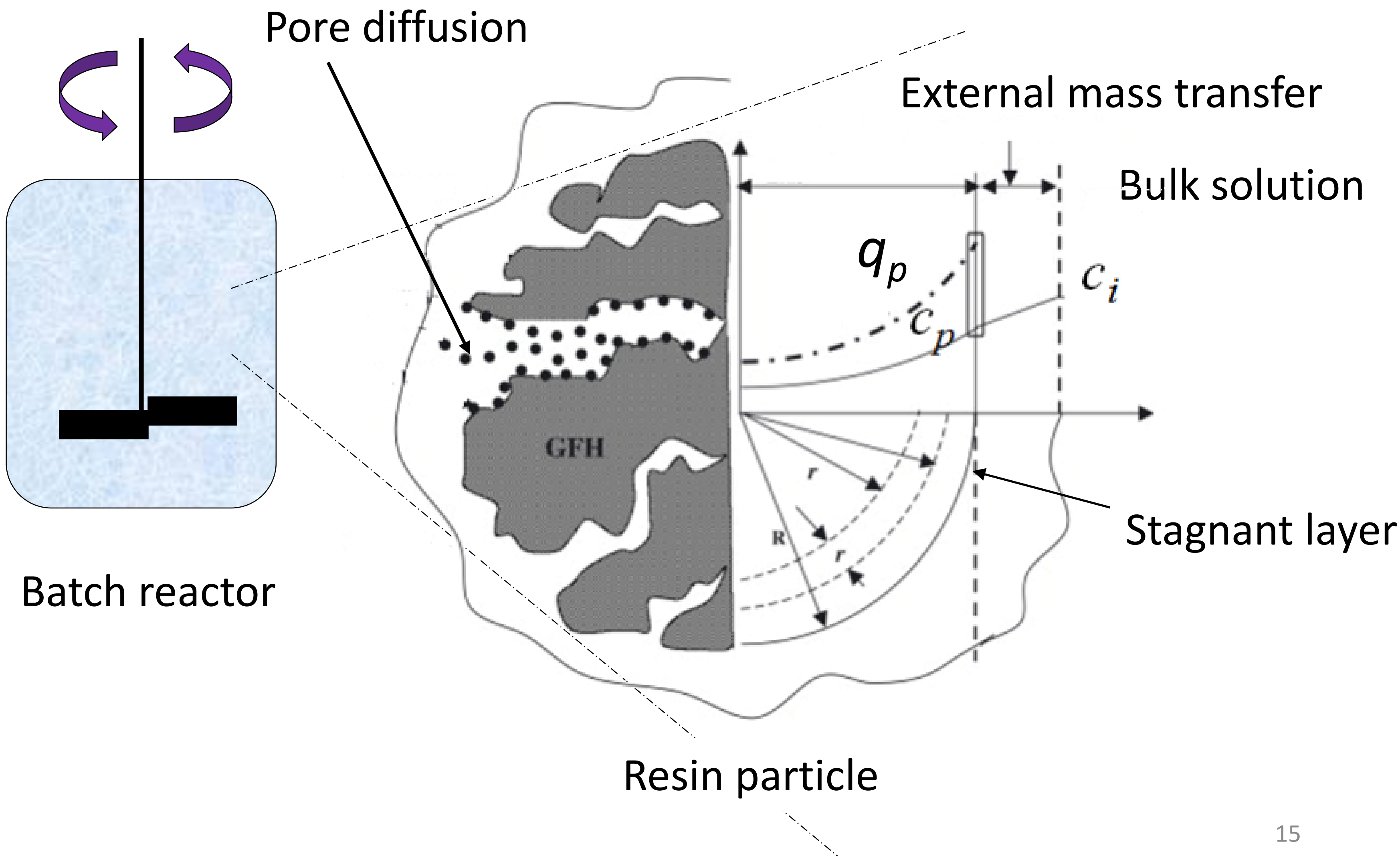
Purolite A835



Reillex 425

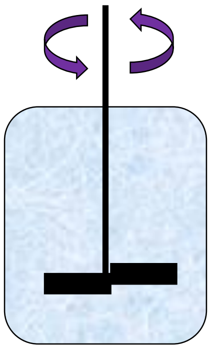


Adsorption kinetics: Mass transfer mechanisms in the transport of solute



Governing equations for batch adsorber kinetics

- The differential mass balance for adsorption of c (z,t) is given by:



Batch reactor

Bulk phase mass balance

$$V\frac{\partial c_i}{\partial t} + \frac{\partial q_i}{\partial t} = 0$$

Intraparticle transport

$$\frac{\partial q_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(D_i\frac{\partial q_i}{\partial r}\right)\right]$$

Isotherm

$$q_i = \frac{q_{mi}K_i c_i}{1 + \sum_j^k K_j c_j}$$

Initial and boundary conditions

$$t = 0:\ c_i = c_{0i}$$

$$0 < r < r_p, t = 0:\ q_i = 0$$

$$r = 0, t > 0:\ \frac{\partial q_i}{\partial r}_{r=0} = 0;$$

$$r = r_p, t > 0:\ D_i\frac{\partial q_i}{\partial r}_{r=r_p} = k_f\left(c_i - c_{pi,r=rp}\right)$$

Governing equations for batch adsorber kinetics

- The differential mass balance for adsorption of c (z,t) is given by:

Particle phase mass balance

$$\frac{\partial q}{\partial t} = D_c \left(\frac{\partial^2 q}{\partial r^2} + \frac{2}{r}\frac{\partial q}{\partial r} \right)$$

Initial and boundary conditions

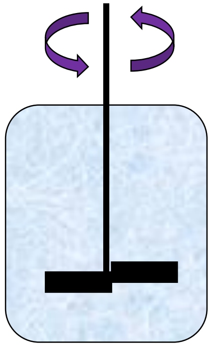
$$q(r,0) = q_0' \qquad \frac{\partial q}{\partial r}_{r=0} = 0$$

$$q(rc,0) = q_0$$

Analytical solution $\alpha < 0.1$

$$1 - \frac{m_t}{m_\infty} \approx \frac{6}{\pi^2} exp^{\left(-\frac{\pi^2 D_c t}{r_c^2}\right)}$$

$$\boxed{\alpha = \frac{C_0 - C_\infty}{C_0}}$$



Batch reactor

Analytical solution $\alpha > 0.1$

$$\frac{m_t}{m_\infty} = 1 - 6\sum_{n=1}^{\infty} \frac{exp^{\left(-\frac{p_n^2 D_c t}{r_c^2}\right)}}{\frac{9\alpha}{(1-\alpha)} + (1-\alpha)p_n^2}$$

$$tan\, p_n = \frac{3p_n}{3 + \left(\frac{1}{\alpha} - 1\right) p_n^2}$$

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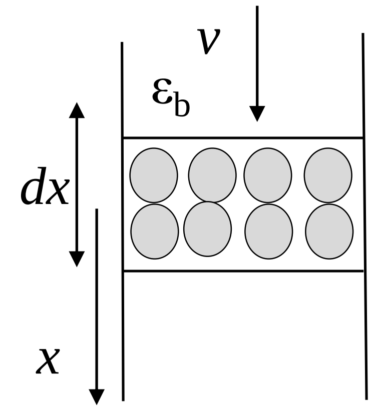

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Bulk phase mass balance

$$-D_{Li}\frac{\partial^2 c_i}{\partial x^2} + v\frac{\partial c_i}{\partial x} + \frac{\partial c_i}{\partial t} + \left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{3}{r_p}k_{fi}\left(c_i - c_{pi,r=rp}\right) = 0$$

Intraparticle transport

$$\varepsilon_p\frac{\partial c_{pi}}{\partial t} + \rho_p\frac{\partial q_{pi}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\varepsilon_p D_{pi}\frac{\partial c_{pi}}{\partial r}\right)\right]$$

Isotherm

$$q_{pi} = \frac{q_{mi}Ki\, c_{pi}}{1+\sum_i^k Ki\, c_{pi}}$$

Initial and boundary conditions

$$0 < x < L, t = 0:\ c_i = 0$$

$$x = 0, t > 0: D_{Li}\frac{\partial^2 c_i}{\partial x^2} = v(c_{ix=0} - c_{0i})$$

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$$0 < r < r_p, t = 0:\ c_{pi} = 0, q_{pi} = 0$$

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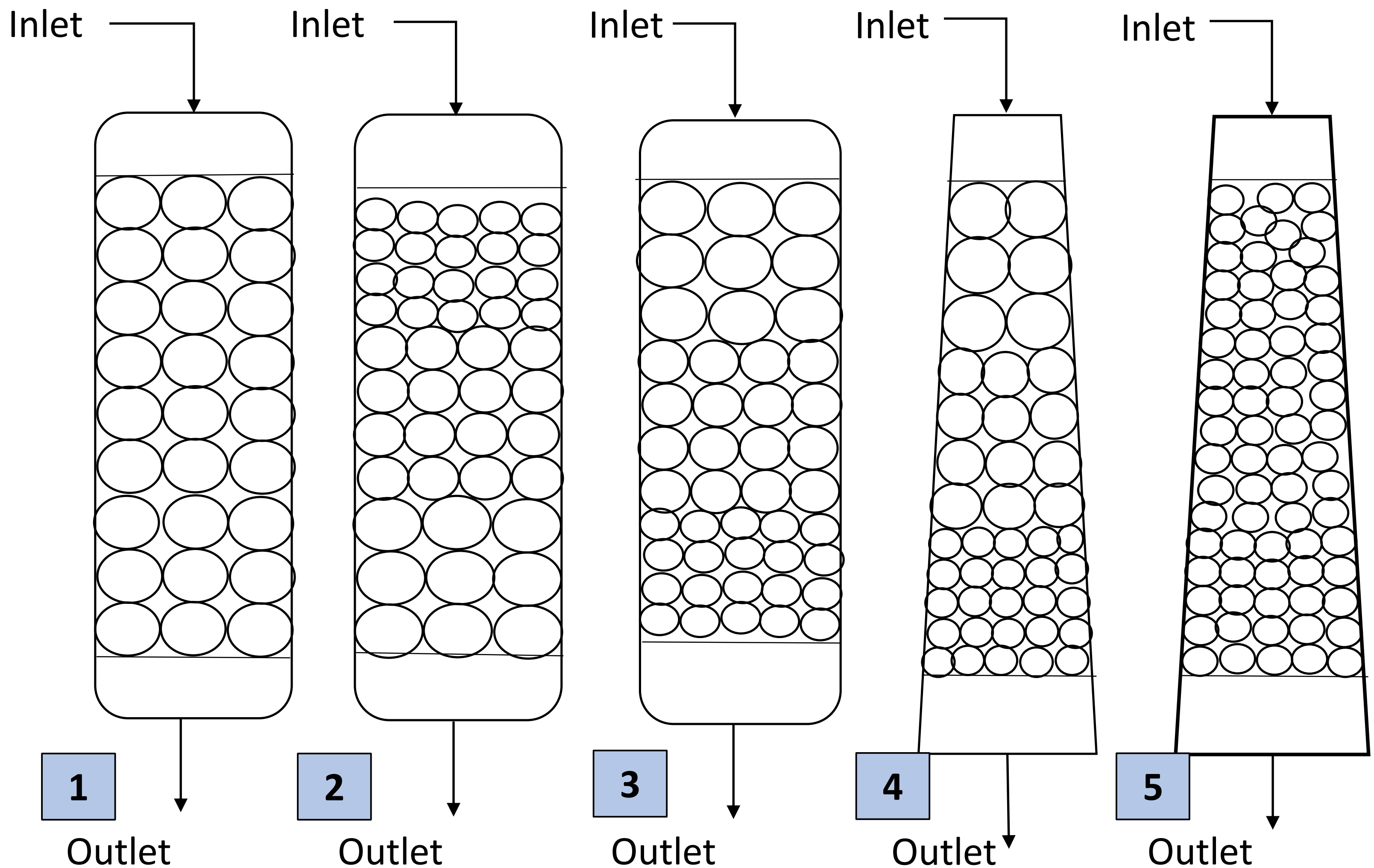
Materials and Methods: Fixed-bed adsorber configurations



Adsorber configurations: (1) conventional cylindrical adsorber (CCA) with single particle size, (2) normally stratified cylindrical adsorber (SCA), (3) reverse stratified cylindrical adsorber, (4) reverse stratified tapered adsorber (RSTA), and (5) tapered bed with single particle size

Physicochemical properties of granular activated carbon and operational parameters

Property	
Particle size (cm)	0.065
Bulk density (g/cm^3)	0.701
Particle porosity	0.66

Operational parameters	
Amount of resin (g)	40
Superficial velocity (cm/min)	2.36
Bed length (cm)	20
Bed diameter (cm)	2.54
Inlet concentration of Acetic acid (g/L)	15
Isotherm constant, a (g/g)	0.186
Isotherm constant, b (L/g)	0.53

Stratified adsorber	
Mesh fraction	Particle size (cm)
18-20	0.092
20-25	0.077
25-30	0.065
30-35	0.055
35-40	0.046

Tapered bed adsorber dimensions	
Bed length (cm)	14.4
Bed diameter top (cm)	2
Bed diameter bottom (cm)	4

Physicochemical properties of Purolite A835 resin and operational parameters

Property	
Particle size (cm)	0.065
Wet particle density (g/cm^3)	1.072
Particle porosity	0.28

Stratified adsorber	
Mesh fraction	Particle size (cm)
20-25	0.077
25-30	0.065
30-35	0.055

Operational parameters	
Amount of resin (g)	62
Superficial velocity (cm/min)	2.36
Bed length (cm)	18
Bed diameter (cm)	2.54
Inlet concentration of Acetic acid (g/L)	15
Maximum adsorption capacity, q_{max} (g/g)	0.27
Isotherm constant, k (L/g)	0.506

Tapered bed adsorber dimensions	
Bed length (cm)	13.25
Bed diameter top (cm)	2.44
Bed diameter bottom (cm)	3.5

pH of Multicomponent studies	
2.8	4.8

Operational parameters

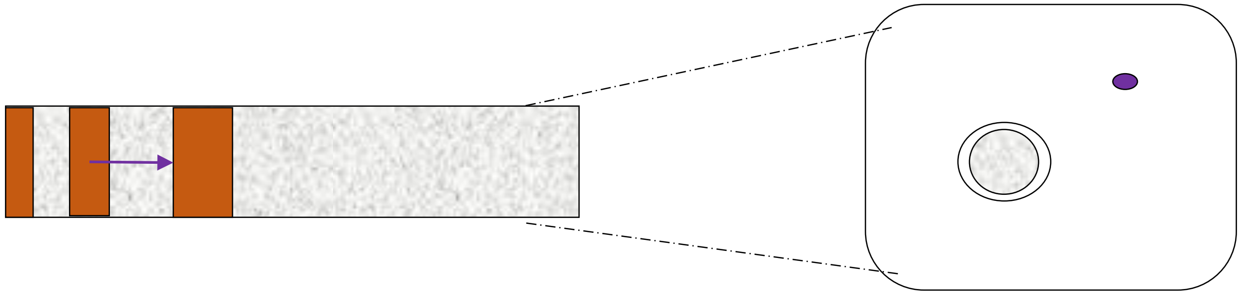
Axial dispersion coefficient
(Suzuki and Smith, 1972)

External mass transfer coefficient
(Dwivedi and Upadhyay, 1977)

Pore diffusion coefficient
(Mackie and Maeres, 1955)

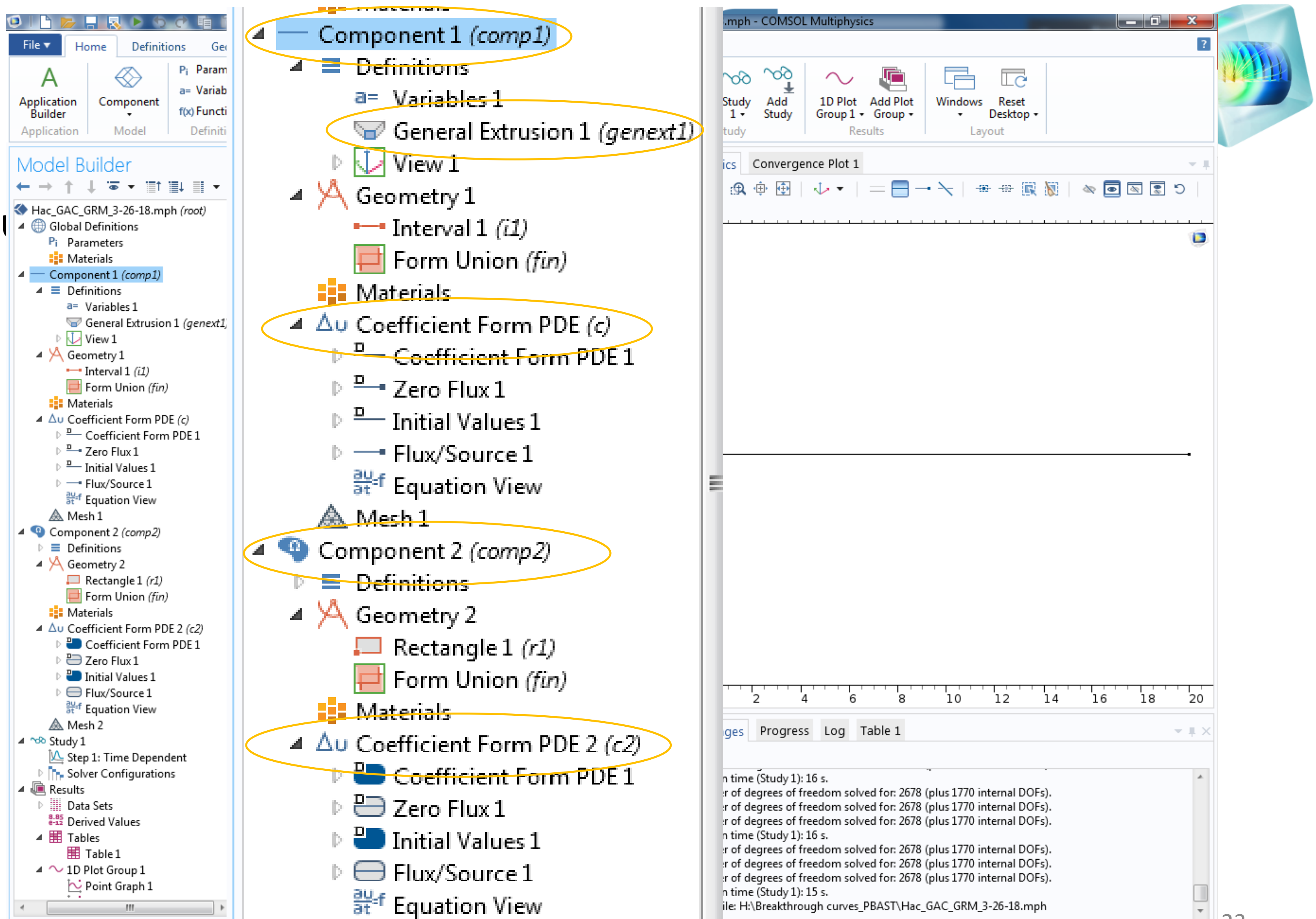
Component	D_L (cm^2/min)	K_f(cm/min)	D_p (*10^4 cm^2/min)
Acetic acid	0.128	0.101	2.7

Component	D_L (cm^2/min)	K_f (cm/min)	D_p (*10^5 cm^2/min)
Acetic acid	0.128	0.018	6.6
Lactic acid	0.095	0.016	2.7



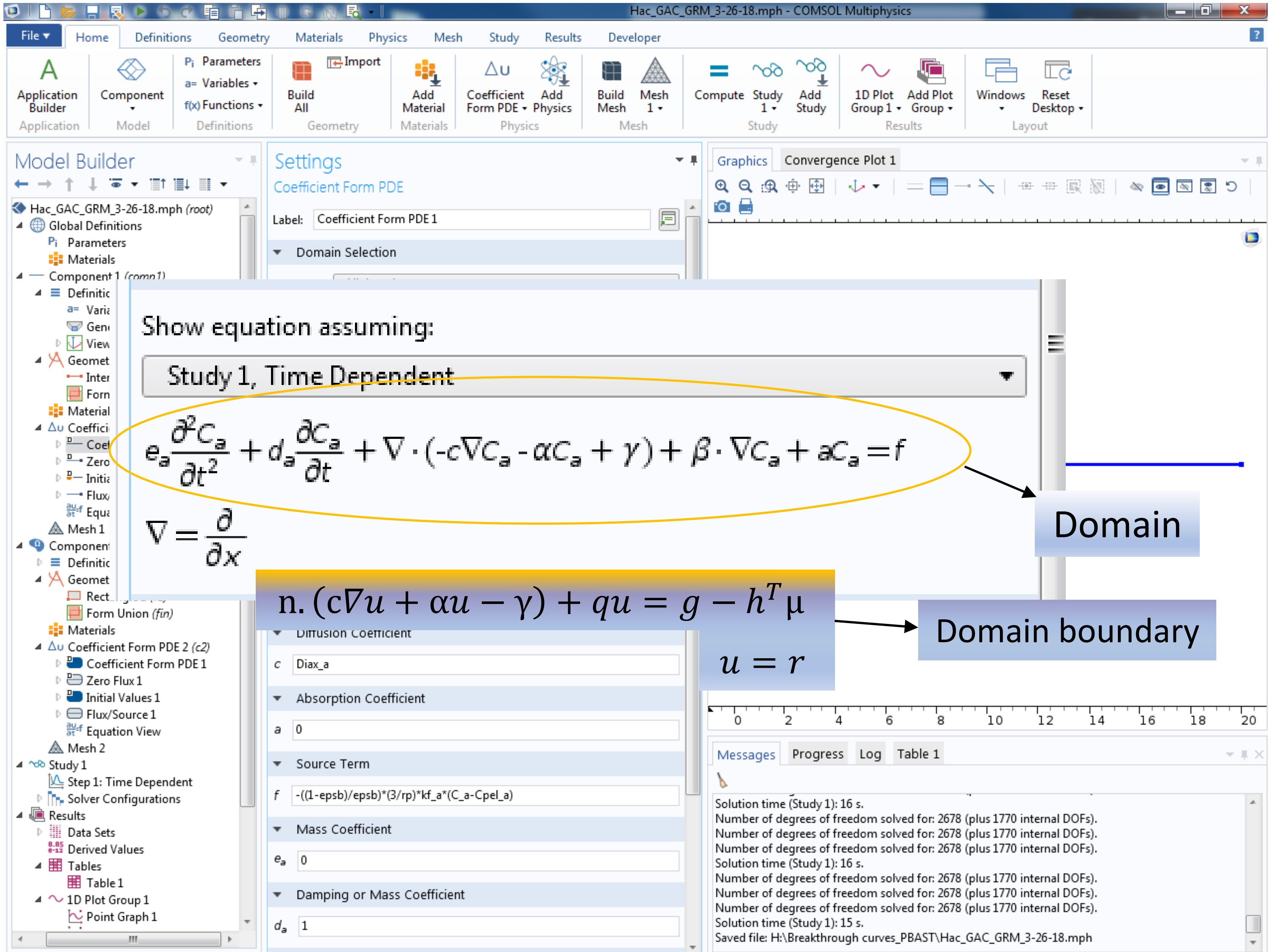
Implementation in COMSOL Multiphysics®

- M



Implementation in COMSOL Multiphysics®

Coefficient form PDE interface in COMSOL Multiphysics®



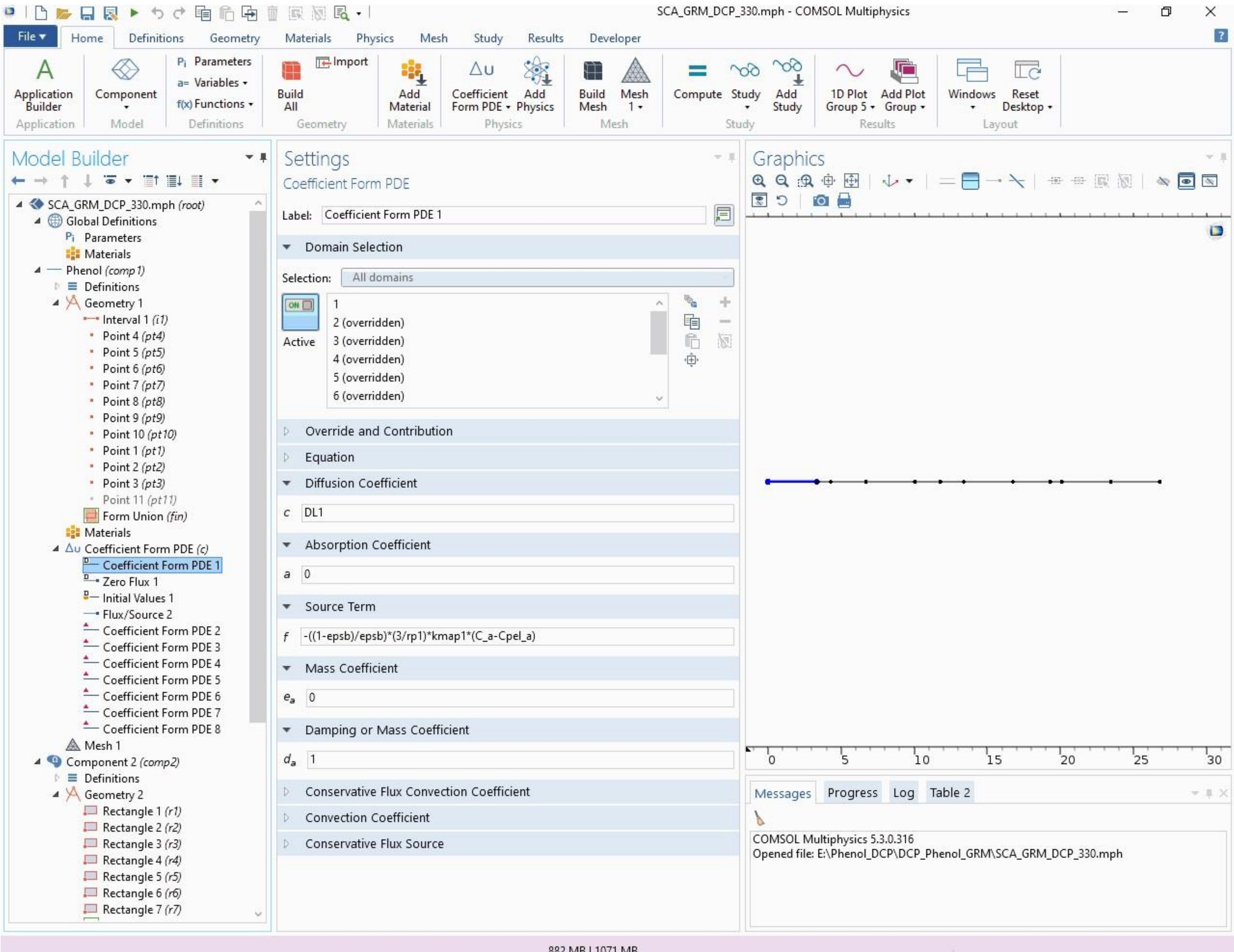

SCA_GRM_DCP_330.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Component
Parameters
Variables
Functions
Build All
Import
Add Material
Coefficient Form PDE
Add Physics
Build Mesh
Mesh 1
Compute
Study
Add Study
1D Plot Group 5
Add Plot Group
Windows
Reset Desktop
Application
Model
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Layout
Model Builder
SCA_GRM_DCP_330.mph (root)
Global Definitions
Parameters
Materials
Phenol (comp1)
Definitions
Geometry 1
Interval 1 (i1)
Point 4 (pt4)
Point 5 (pt5)
Point 6 (pt6)
Point 7 (pt7)
Point 8 (pt8)
Point 9 (pt9)
Point 10 (pt10)
Point 1 (pt1)
Point 2 (pt2)
Point 3 (pt3)
Point 11 (pt11)
Form Union (fin)
Materials
Coefficient Form PDE (c)
Coefficient Form PDE 1
Zero Flux 1
Initial Values 1
Flux/Source 2
Coefficient Form PDE 2
Coefficient Form PDE 3
Coefficient Form PDE 4
Coefficient Form PDE 5
Coefficient Form PDE 6
Coefficient Form PDE 7
Coefficient Form PDE 8
Mesh 1
Component 2 (comp2)
Definitions
Geometry 2
Rectangle 1 (r1)
Rectangle 2 (r2)
Rectangle 3 (r3)
Rectangle 4 (r4)
Rectangle 5 (r5)
Rectangle 6 (r6)
Rectangle 7 (r7)
Settings
Coefficient Form PDE
Label: Coefficient Form PDE 1
Domain Selection
Selection: All domains
Active
1
2 (overridden)
3 (overridden)
4 (overridden)
5 (overridden)
6 (overridden)
Override and Contribution
Equation
Diffusion Coefficient
c DL1
Absorption Coefficient
a 0
Source Term
f -((1-epsb)/epsb)*(3/rp1)*kmap1*(C_a-Cpel_a)
Mass Coefficient
ea 0
Damping or Mass Coefficient
da 1
Conservative Flux Convection Coefficient
Convection Coefficient
Conservative Flux Source
Graphics
0
5
10
15
20
25
30
Messages
Progress
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Table 2
COMSOL Multiphysics 5.3.0.316
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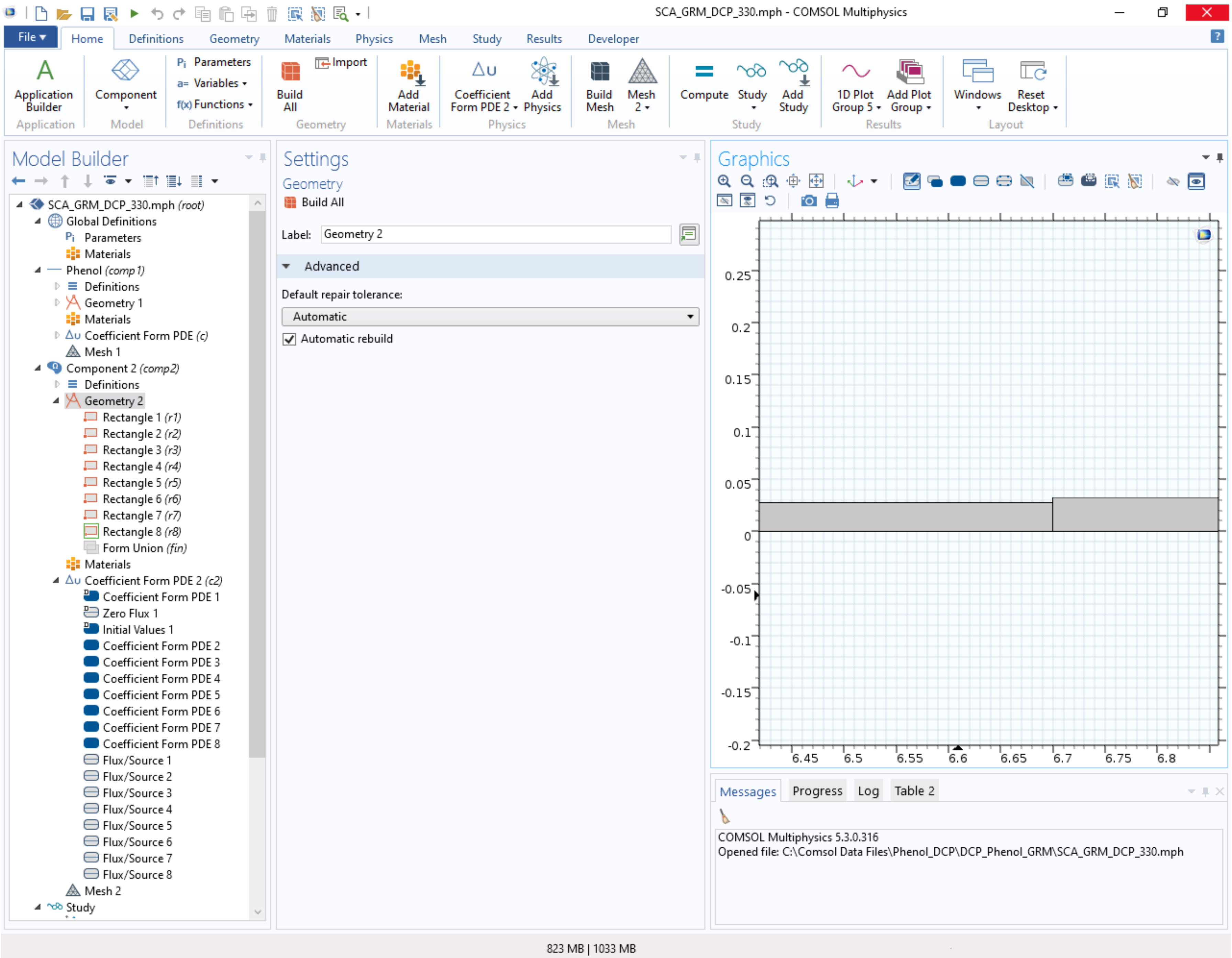
SCA_GRM_DCP_330.mph - COMSOL Multiphysics
File
Home
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Parameters
Variables
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Build All
Import
Geometry
Add Material
Materials
Coefficient Form PDE 2
Add Physics
Physics
Build Mesh
Mesh 2
Mesh
Compute
Study
Add Study
Study
1D Plot Group 5
Add Plot Group
Results
Windows
Reset Desktop
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Model Builder
SCA_GRM_DCP_330.mph (root)
Global Definitions
Parameters
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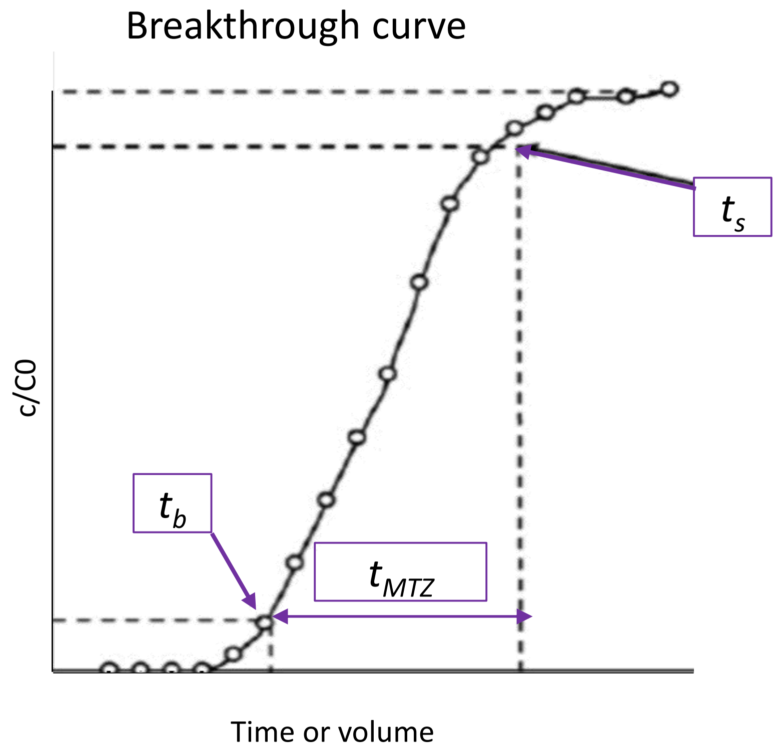
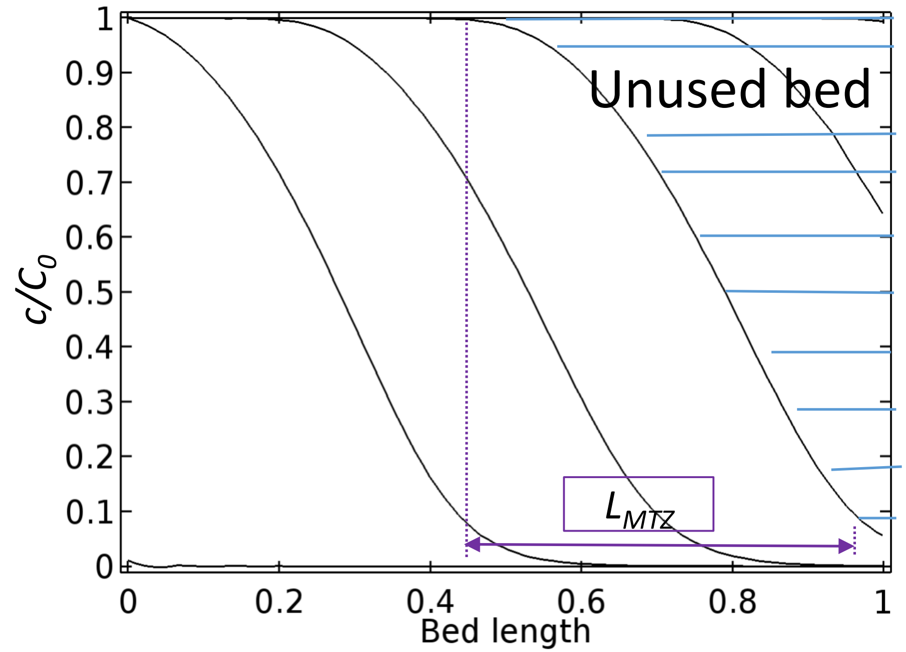
Definitions
Geometry 1
Materials
Coefficient Form PDE (c)
Mesh 1
Component 2 (comp2)
Definitions
Geometry 2
Rectangle 1 (r1)
Rectangle 2 (r2)
Rectangle 3 (r3)
Rectangle 4 (r4)
Rectangle 5 (r5)
Rectangle 6 (r6)
Rectangle 7 (r7)
Rectangle 8 (r8)
Form Union (fin)
Materials
Coefficient Form PDE 2 (c2)
Coefficient Form PDE 1
Zero Flux 1
Initial Values 1
Coefficient Form PDE 2
Coefficient Form PDE 3
Coefficient Form PDE 4
Coefficient Form PDE 5
Coefficient Form PDE 6
Coefficient Form PDE 7
Coefficient Form PDE 8
Flux/Source 1
Flux/Source 2
Flux/Source 3
Flux/Source 4
Flux/Source 5
Flux/Source 6
Flux/Source 7
Flux/Source 8
Mesh 2
Study
Settings
Geometry
Build All
Label: Geometry 2
Advanced
Default repair tolerance:
Automatic
Automatic rebuild
Graphics
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
6.45
6.5
6.55
6.6
6.65
6.7
6.75
6.8
Messages
Progress
Log
Table 2
COMSOL Multiphysics 5.3.0.316
Opened file: C:\Comsol Data Files\Phenol_DCP\DCP_Phenol_GRM\SCA_GRM_DCP_330.mph
823 MB | 1033 MB

Bed capacity utilization



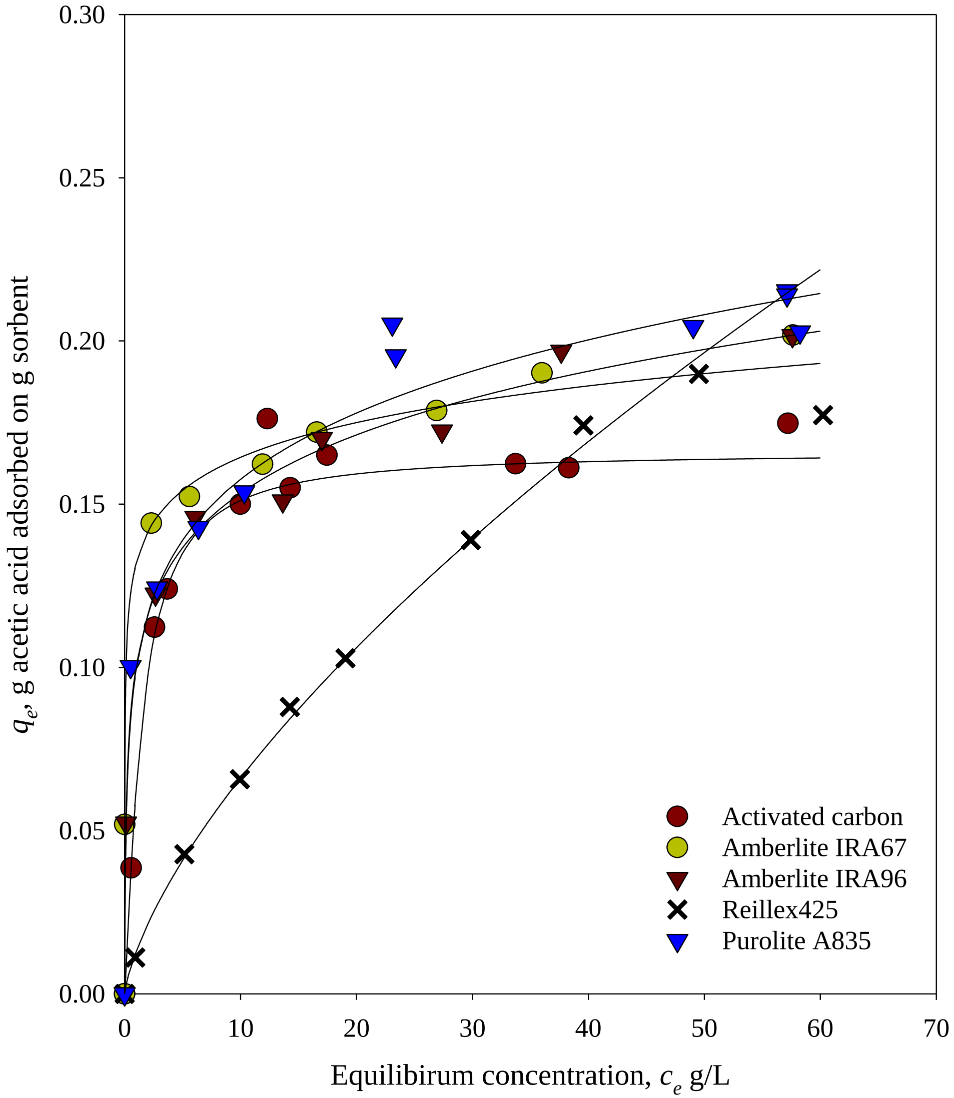


$$L_{MTZ} = U_{sh} t_{MTZ}$$

$$U_{sh} = \frac{V}{\left(1 + \frac{(1-\varepsilon_b)}{\varepsilon_b} \rho_p \frac{q_0}{C_0}\right)}$$

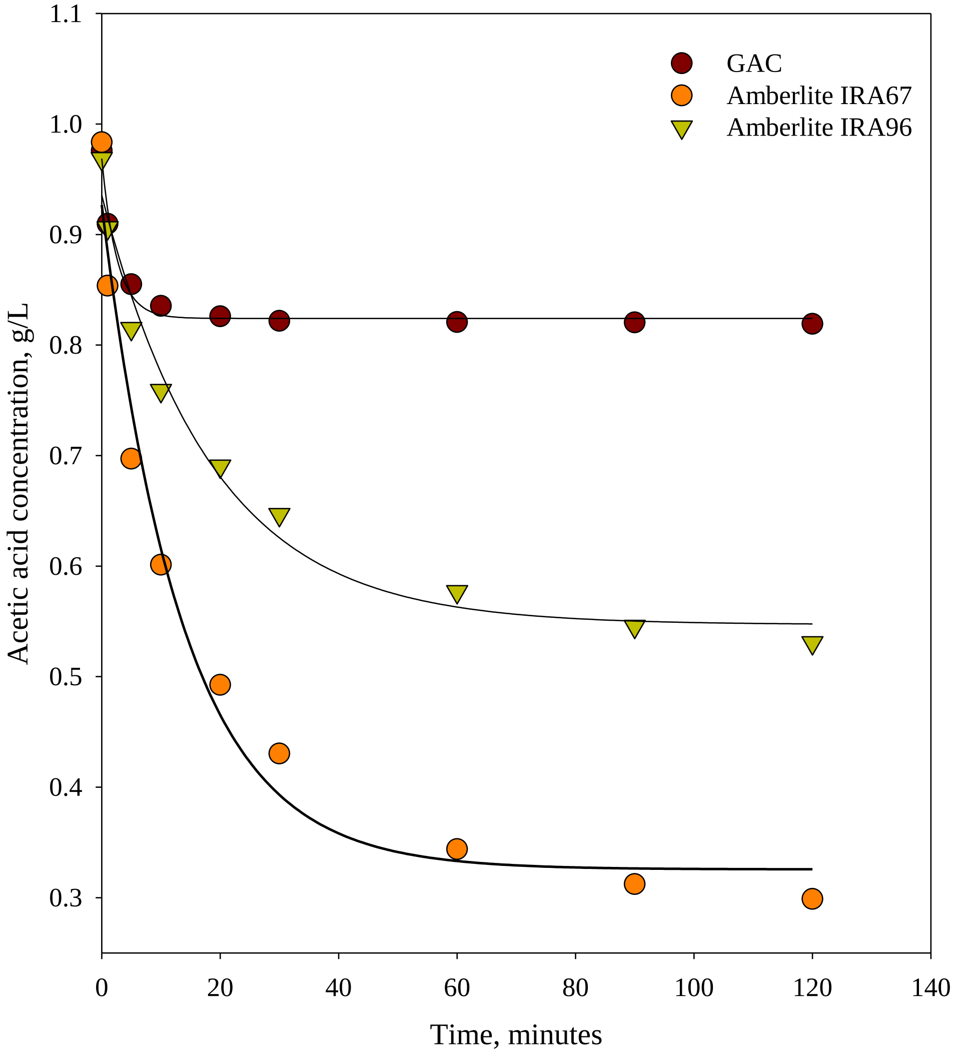
$$fractional\ bed\ capacity\ utilization = 1 - 0.5 * \frac{L_{MTZ}}{L}$$

Single component adsorption equilibria of acetic acid: Experimental data



- Uptake capacities of weak base resins were higher compared to GAC
- Purolite A835 had highest sorption capacity among the sorbents

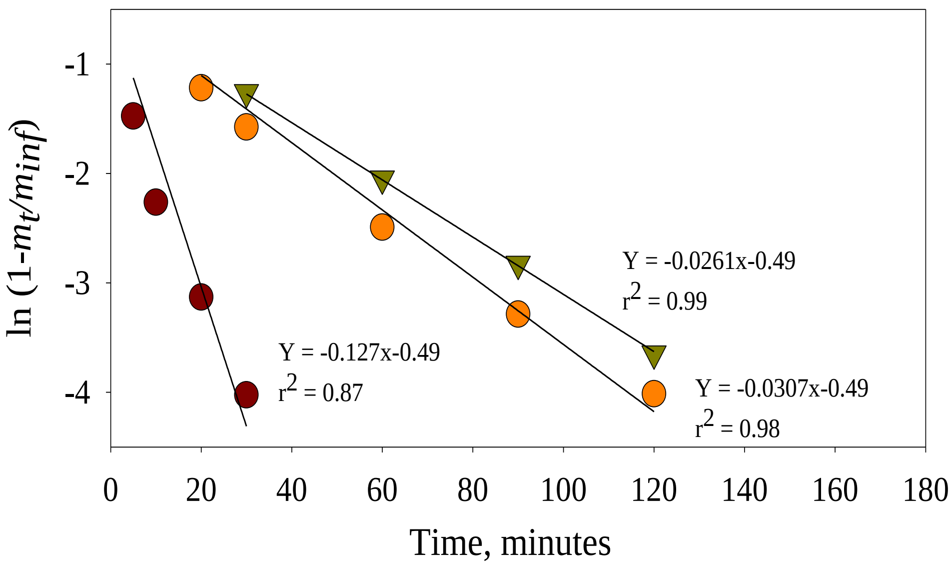
Adsorption kinetics of acetic acid on GAC and resins: Experimental data



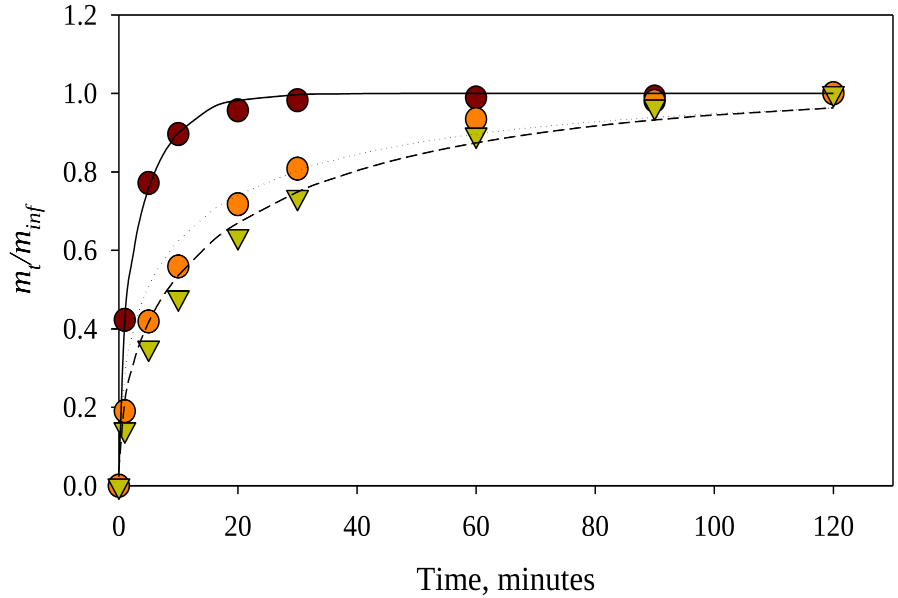
- All sorbents show a common pattern of rapid decrease in first few minutes
- It is followed by little or no change in concentration over the time range studied

Adsorption kinetics of acetic acid on GAC and resins: Kinetic parameters

Linearized equation of infinite bath system



Nonlinear finite bath equation



● Activated carbon ● Amberlite IRA67 ▼ Amberlite IRA96

- External mass transfer coefficient, k_f, is determined using: $k_f = \frac{\rho_p r_p}{3W} \frac{ln\left(\frac{C_0}{C}\right)}{t}$

- Intraparticle diffusivity, D_c, is obtained using linearized equation obtained for infinite bath system and nonlinear finite bath system equation

Adsorption kinetics of acetic acid on GAC and resins: Kinetic parameters

	GAC	**Amberlite IRA67**	**Amberlite IRA96**
k_f (cm/sec)	1.98E-3	5.33E-3	2.72E-3
D_c (cm^2/sec) Equation (4.7)	1.59E-7	0.530E-7	0.537E-7
D_c (cm^2/sec) Equation (4.9)	1.94E-7	0.158E-7	0.304E-7
ARE	1.17	11.23	11.08

- k_f was lower for GAC because of its low sorption capacity and the low sorbent to solute ratio (0.375 g/L) used to effectively suspend it

- k_f of Amberlite IRA67 was higher than that of the Amberlite IRA96

- For GAC, α was 0.15, and D_c obtained from the finite system equation is 22% higher than that from the infinite volume system equation.

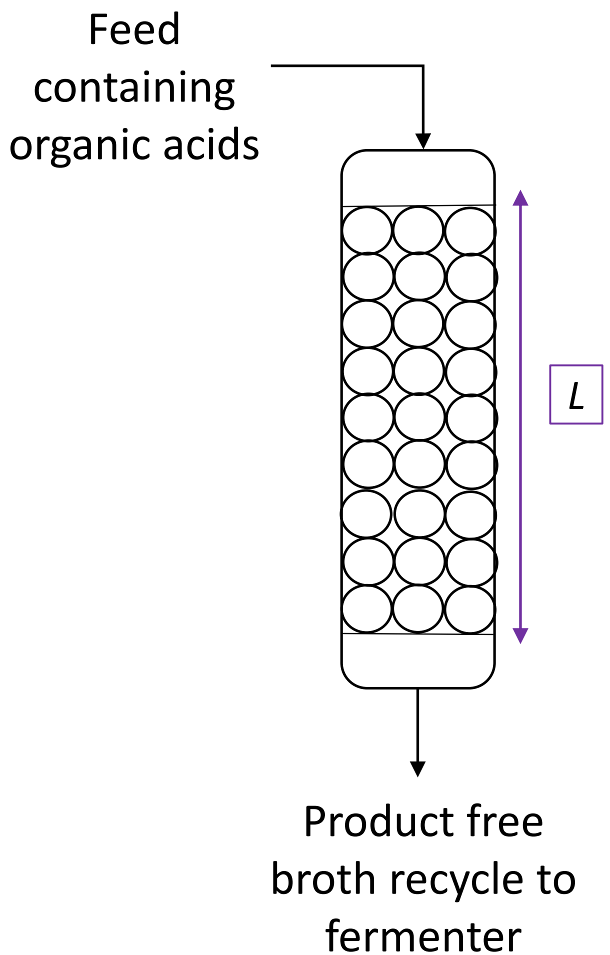
- But, D_c obtained for Amberlite IRA67 and Amberltie IRA96 resins are much more different from each other as α values were 0.69 and 0.45, respectively.

Single component adsorption dynamics in stratified beds

Single component adsorption dynamics

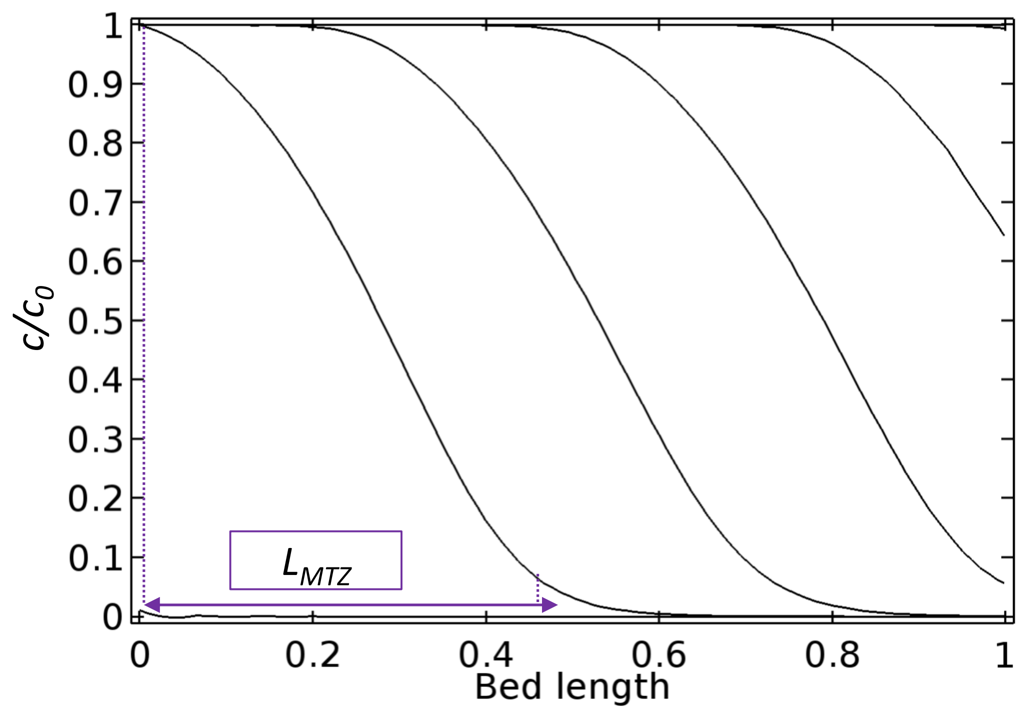
Cylindrical column

Single adsorbent particle size



Concentration profile along the bed length

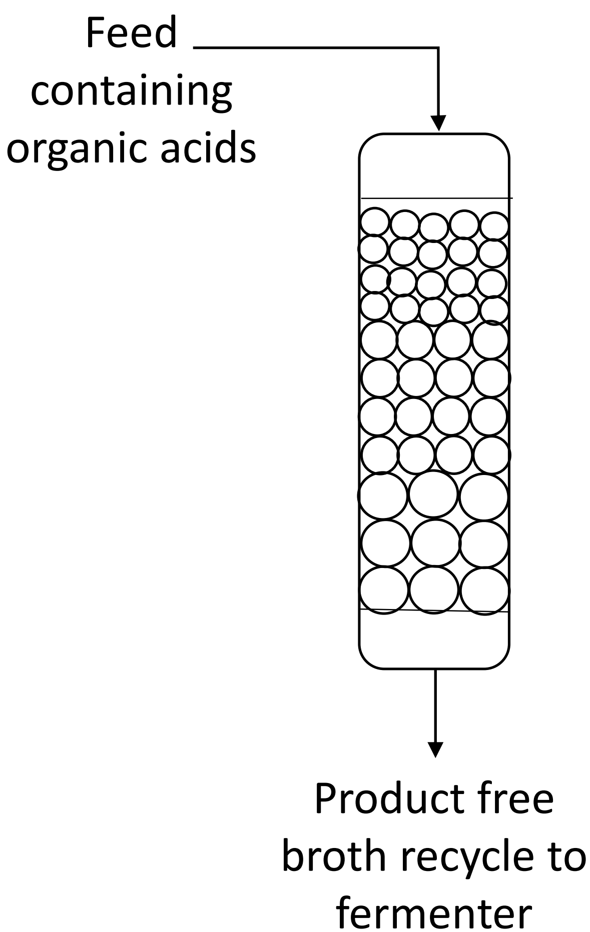
Constant pattern solute front



Single component adsorption dynamics

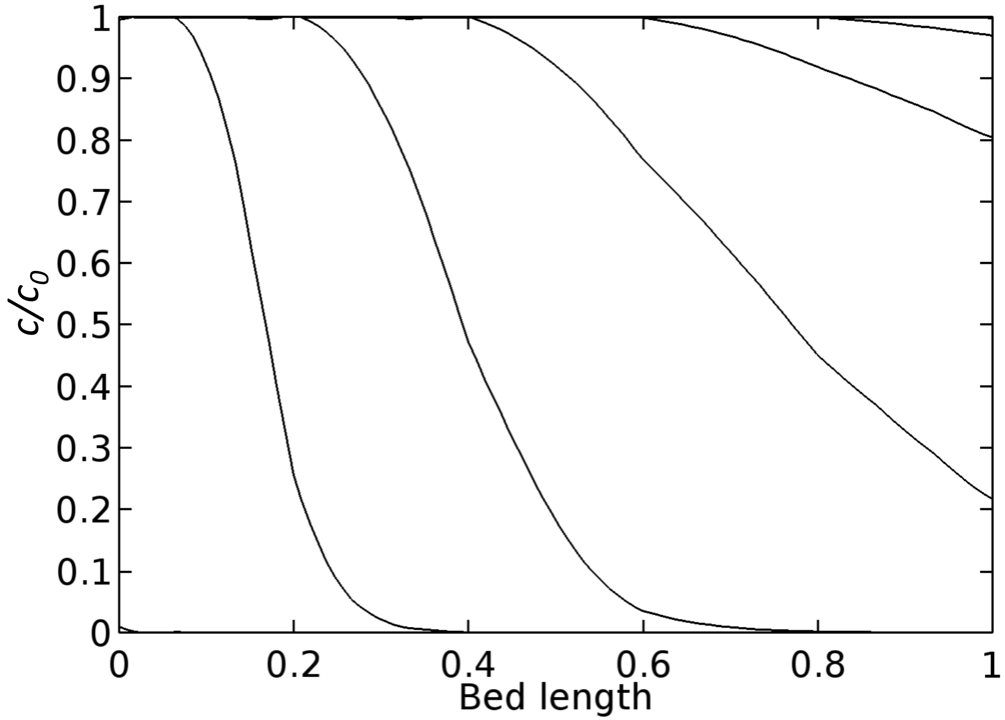
Cylindrical column

Normal stratification



Concentration profile along the bed length

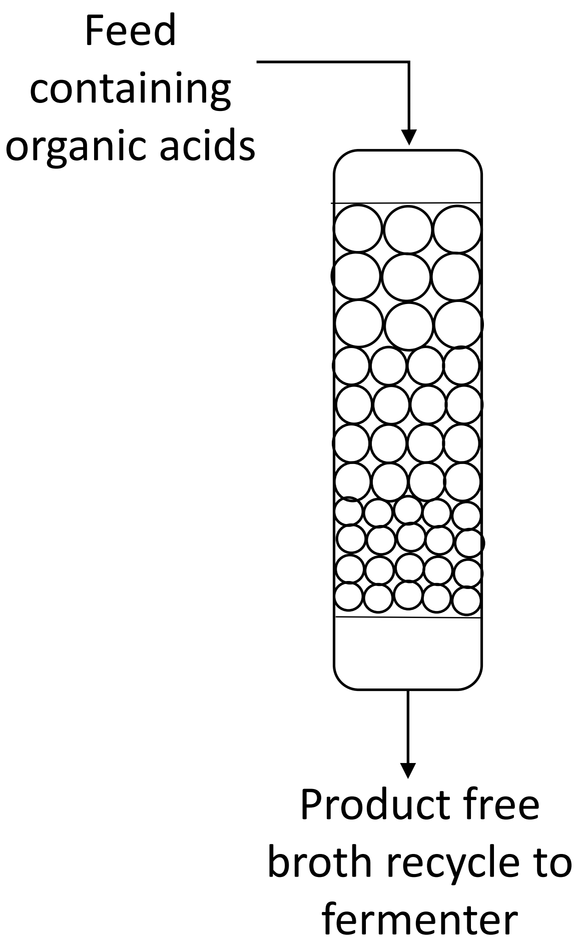
Dispersive solute front



Single component adsorption dynamics

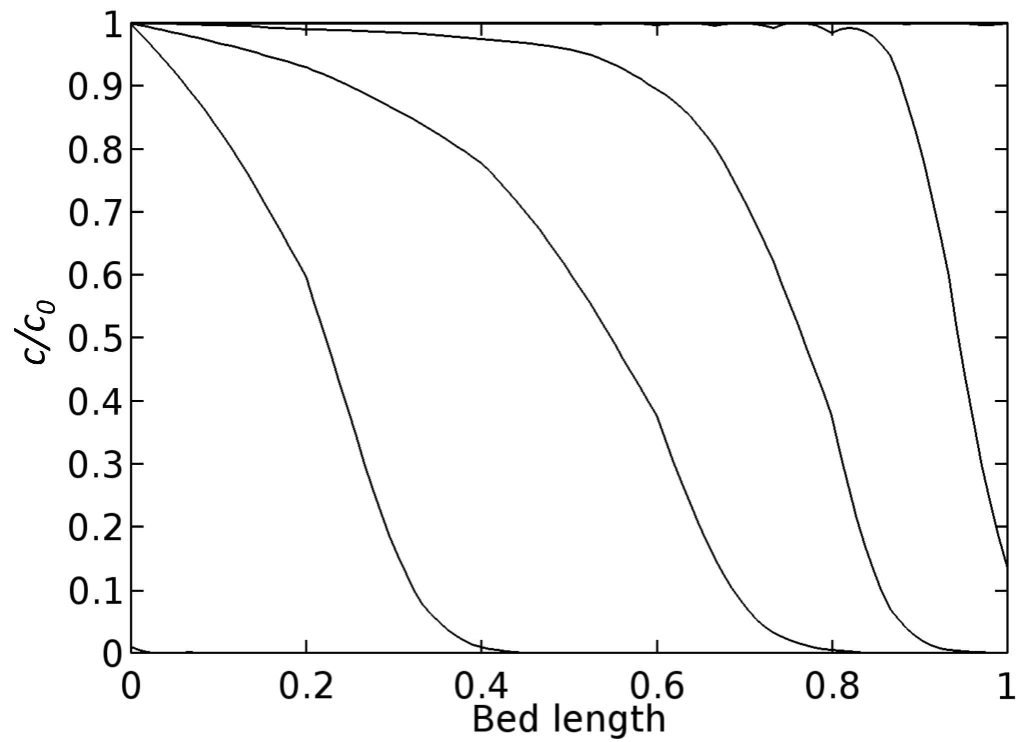
Cylindrical column

Reverse stratification



Concentration profile along the bed length

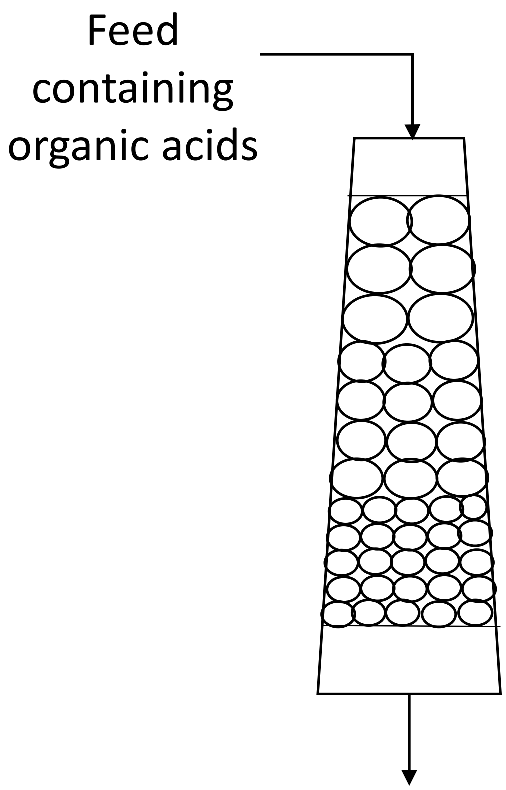
Sharpening solute front



Single component adsorption dynamics

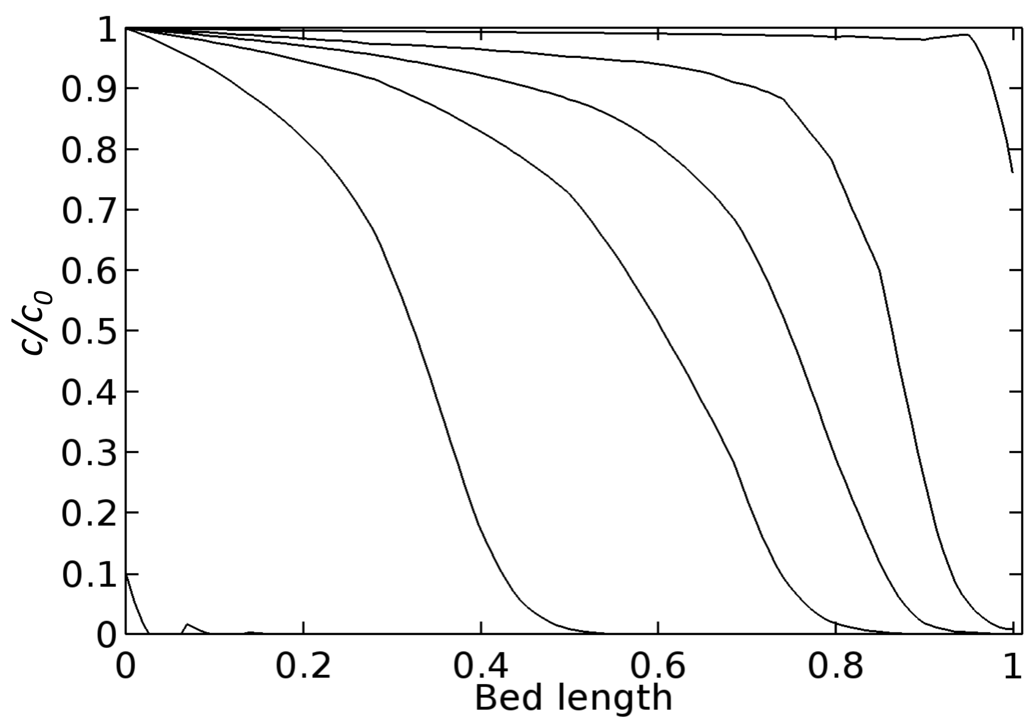
Tapered column

Reverse stratification



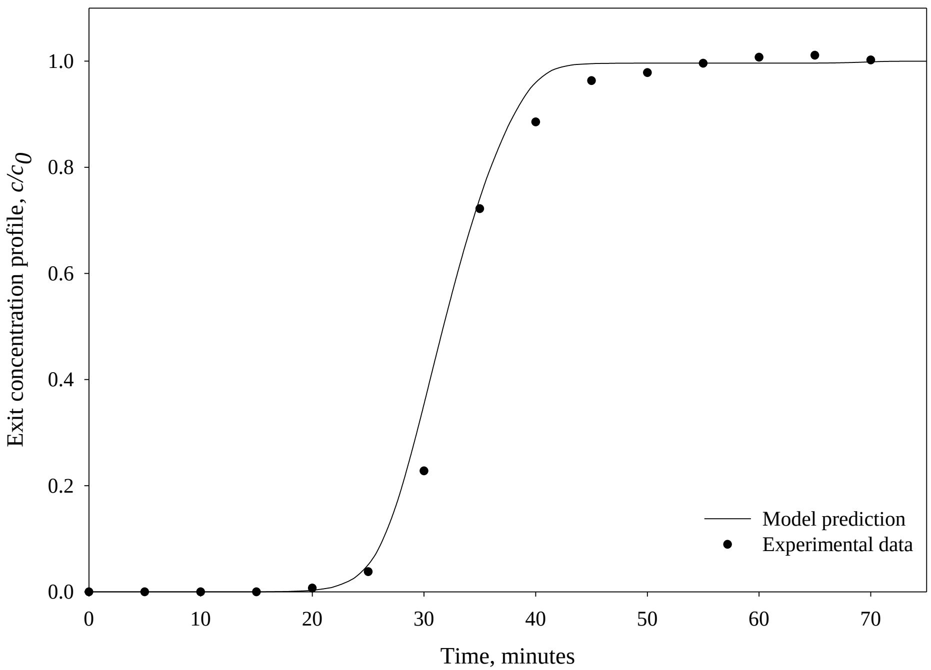
Concentration profile along the bed length

Sharpening solute front

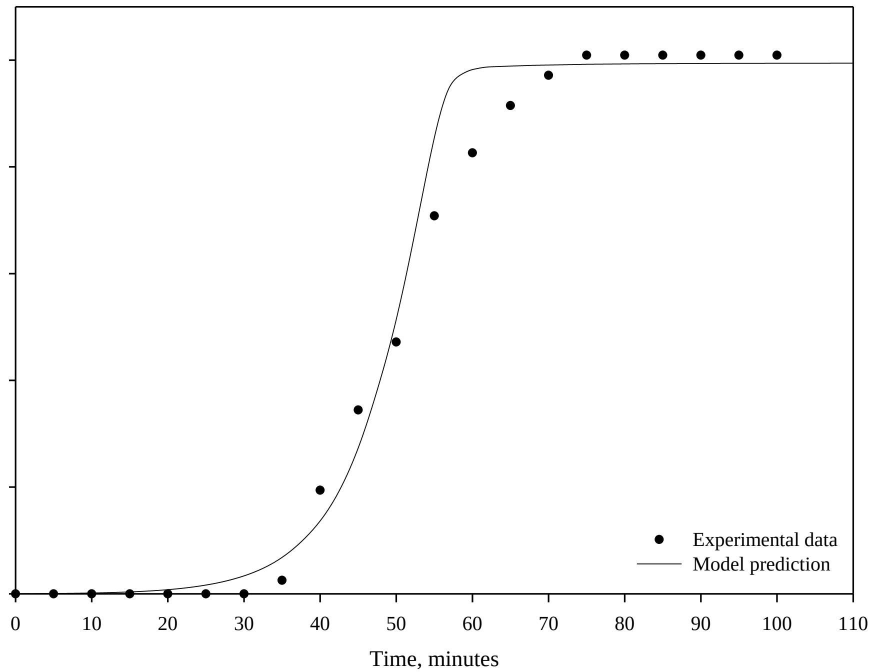


Breakthrough curve analysis

Cylindrical adsorber with single adsorbent particle size



GAC

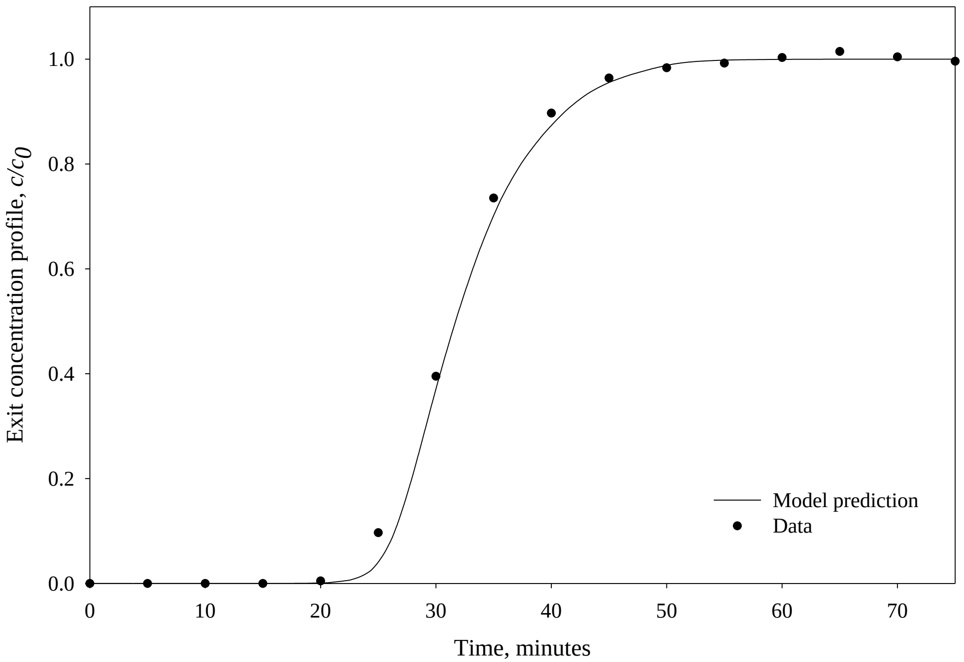


Purolite A835

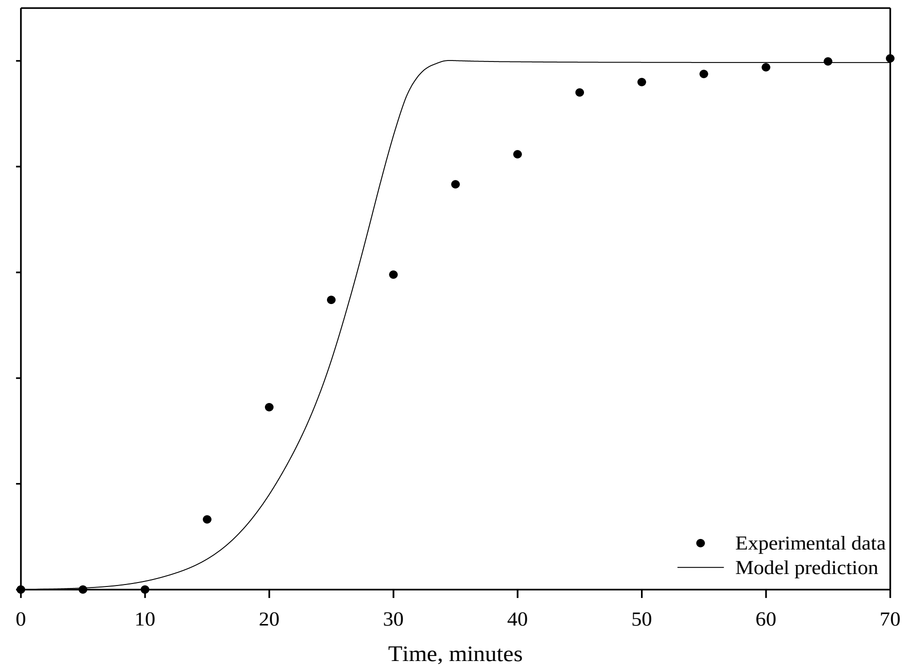
- Constant pattern solute front develops
- Mass transfer effects are uniform along bed length

Breakthrough curve analysis

Cylindrical adsorber with normally stratified adsorbent



GAC

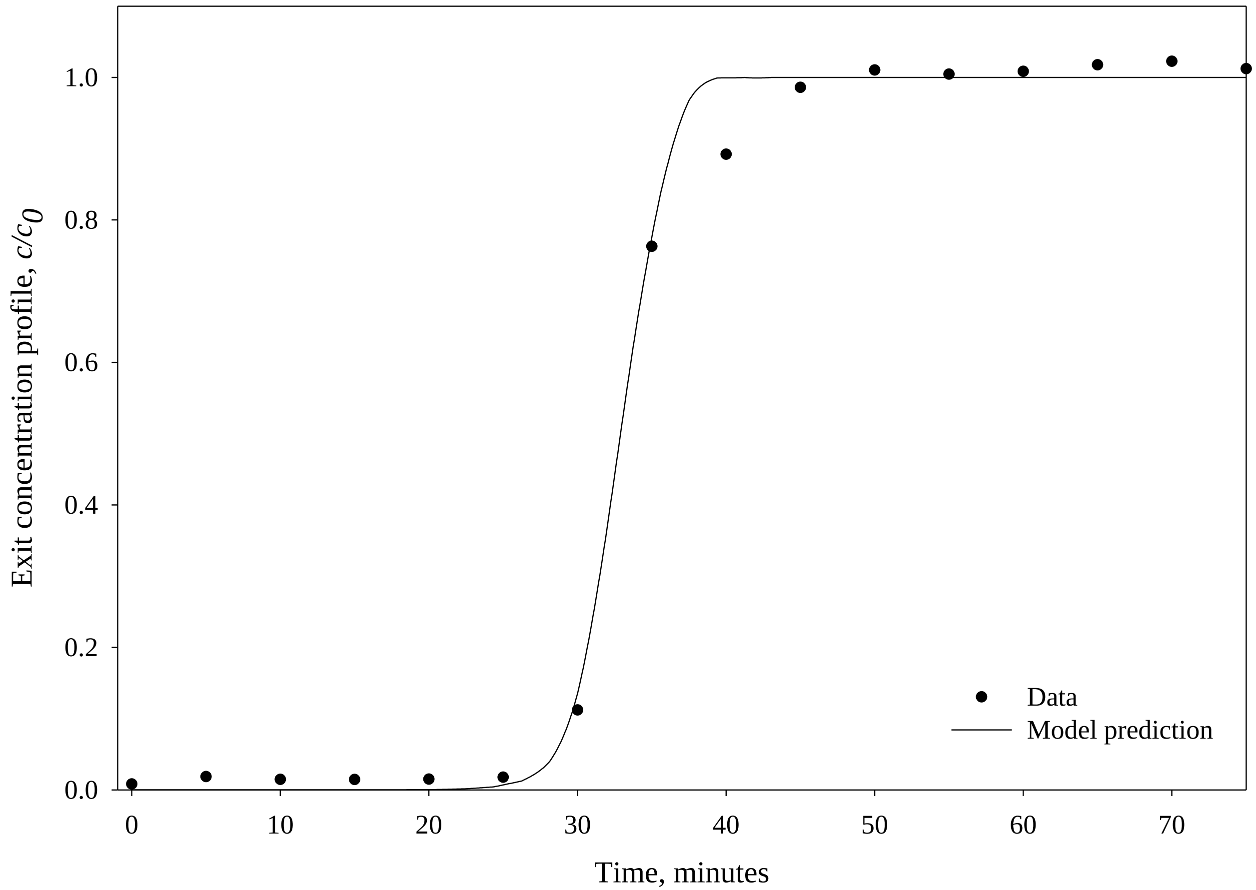


Purolite A835

- Solute front disperses along the bed length
- t_b decreases and t_s increases

Breakthrough curve analysis

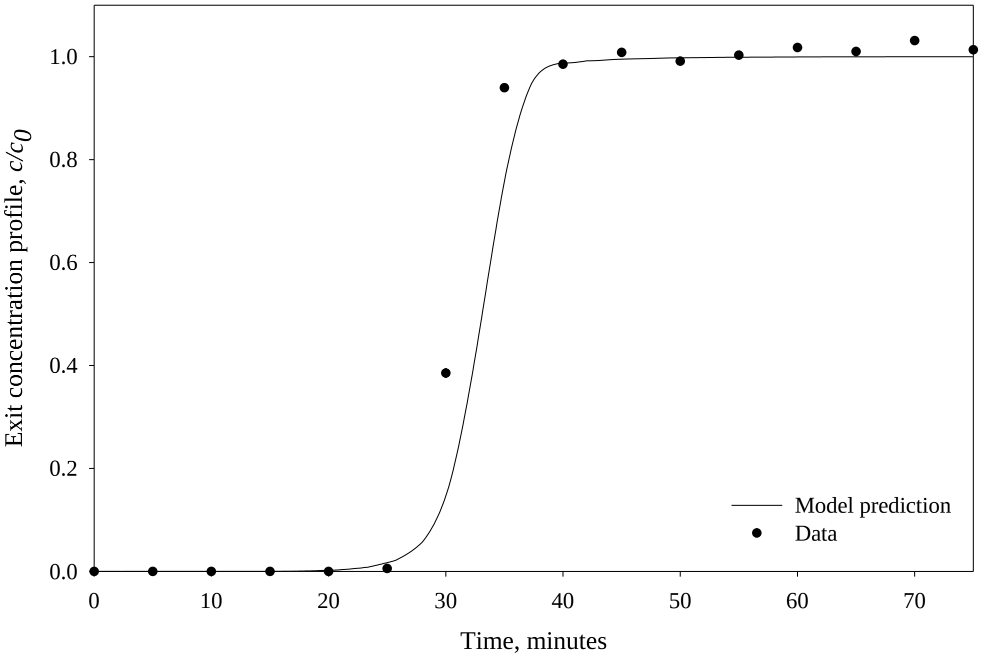
Cylindrical adsorber with reverse stratified adsorbent (GAC)



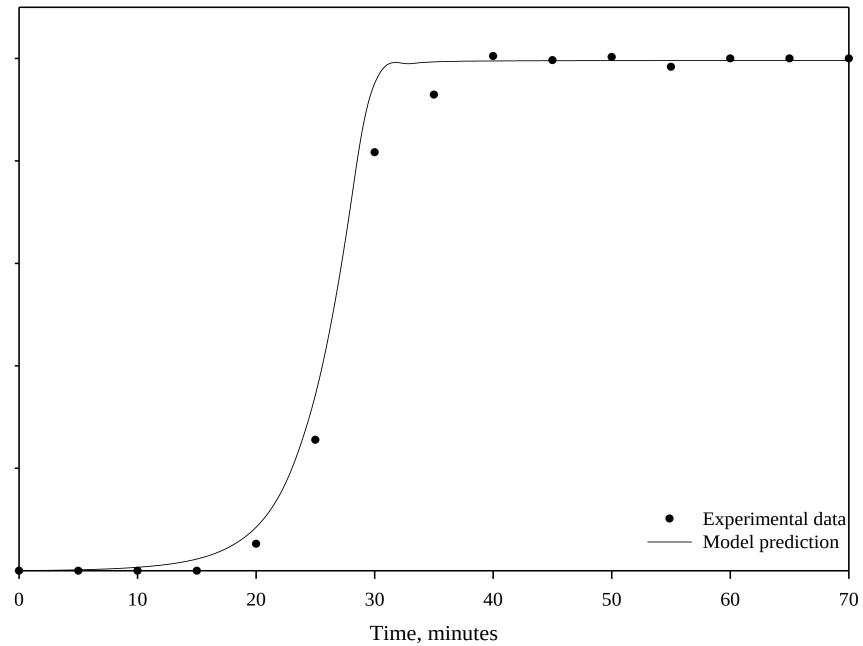
- Solute front sharpens along the bed length
- t_b increases more compared to the increase in t_s

Breakthrough curve analysis

Tapered adsorber with reverse stratified adsorbent



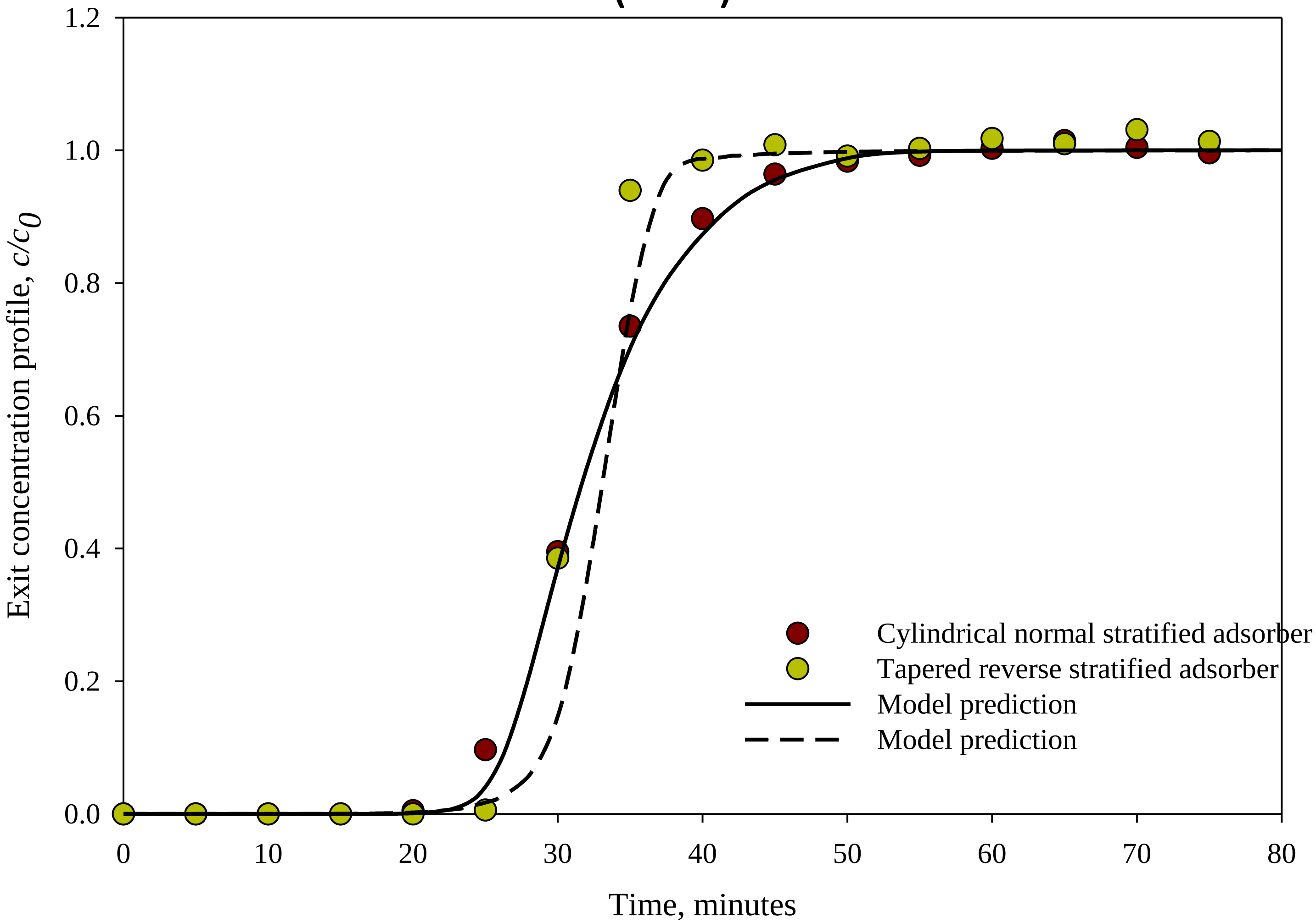
GAC



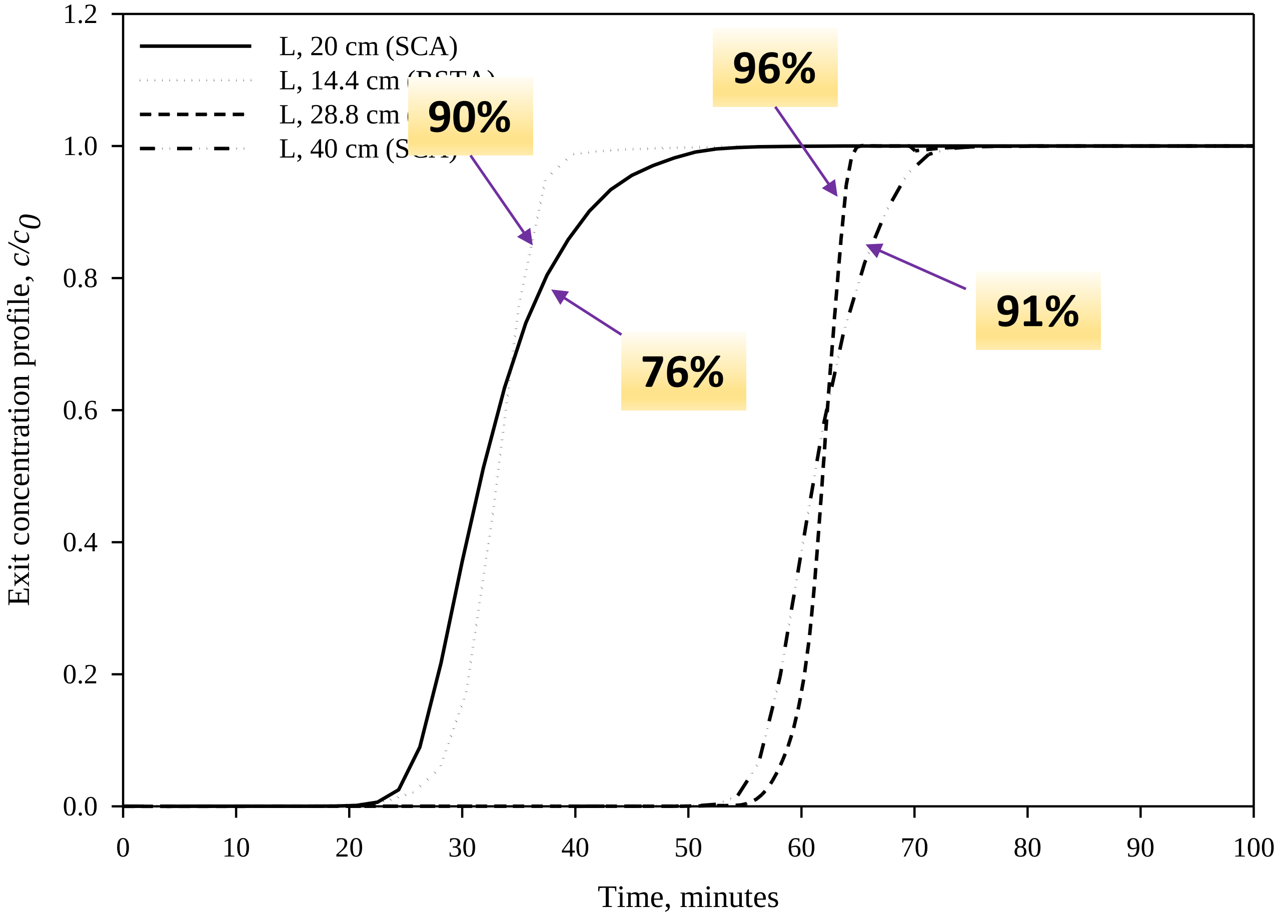
Purolite A835

- Solute front sharpens along the bed length
- Combined effect of decrease in shock front velocity and increase in mass transfer effects

Comparison of exit concentration profiles: Cylindrical adsorber with normal stratified adsorbent and tapered adsorber with reverse stratified adsorbent (GAC)



Comparison of exit concentration profiles: SCA and RSTA with 5 layers of adsorbent particles at double bed length (GAC)



- Double bed length is required for SCA to match the performance of RSTA
- RSTA will require lower adsorbent inventory and reduces the total cost

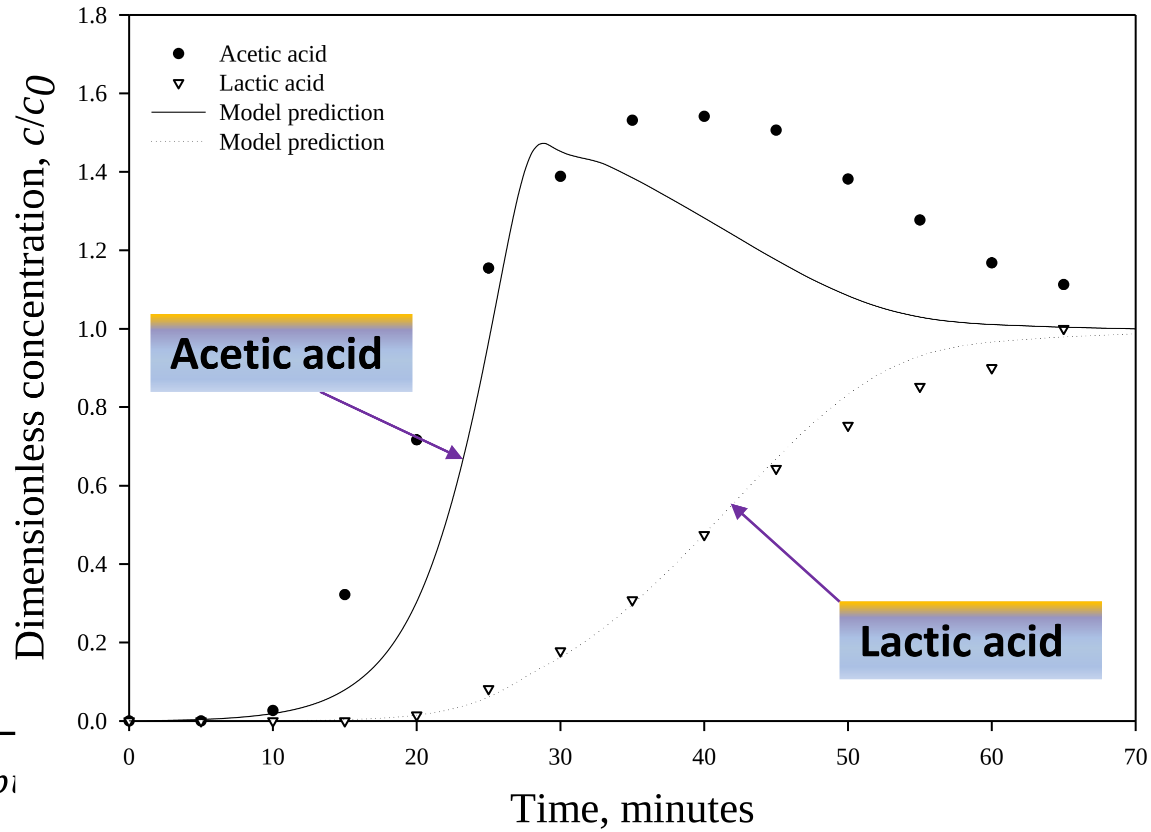
Comparison of shock front velocities and MTZ lengths for various packed bed configurations (GAC)

Experimental parameters	**Cylindrical adsorber - single particle size**	**Normal stratified cylindrical bed**	**Reverse stratified cylindrical bed**	**Reverse stratified tapered bed**
t_b, min	24.8	23.3	27.6	26
t_s, min	39.3	42.5	43	35
t_{MTZ}, min	14.5	19.2	15.4	9
U_{sh}, cm/min	0.612	0.511	0.445	0.308
L_{MTZ}, cm	8.874	9.81	6.85	2.77
Fractional bed capacity utilization	0.78	0.76	0.82	0.90
Fractional bed capacity utilization at double bed length		0.91		0.96

Multicomponent adsorption dynamics

Breakthrough profiles for mixed acid: pH 2.8

Lactic acid C_0 = 15 g/L, Acetic acid C_0 = 6 g/L



$$q_{pi} = \frac{q_{mi} Ki\ c_{pi}}{1 + \sum_i^k Ki\ c_{pi}}$$

- Competitive effect of organic acids on Purolite A835 resin
- Roll-over effect occurs and exit concentration of acetic acid is 1.6 times inlet concentration

Conclusion

- The recovery of organic acids from aqueous solutions was modeled using the General Rate Model that considers external and intraparticle diffusion resistances and nonlinear adsorption isotherm
- COMSOL Multiphysics software was found to be an effective tool for process modeling of batch and fixed-bed adsorbers.
- Process modeling of stratified beds was effectively implemented using COMSOL software
- Kinetic parameters estimated from batch studies gave good predictions for the experimental data
- Reverse stratified tapered adsorber shows higher bed capacity utilization compared to other configurations
- COMSOL implementation of multicomponent adsorption dynamics correctly predicted roll over effects of components