



Loxoprofen SMB (Simulated Moving Bed) Simulation

Loxoprofen

- Loxoprofen {2-[4-(2-oxocyclopentylmethyl)phenyl]-propionic acid}

- 화학구조





서론

- Aspen chromatography를 이용한 시뮬레이션
- MTC(mass transfer coefficient)값 변화
- 전산모사 결과



Linear model

- The linear isotherm is expressed as :

$$W_A = N_A C_A \qquad W_B = N_B C_B$$

- ◆ A is the more adsorbed component
- ◆ B is the less adsorbed component

Starting

- From open menu

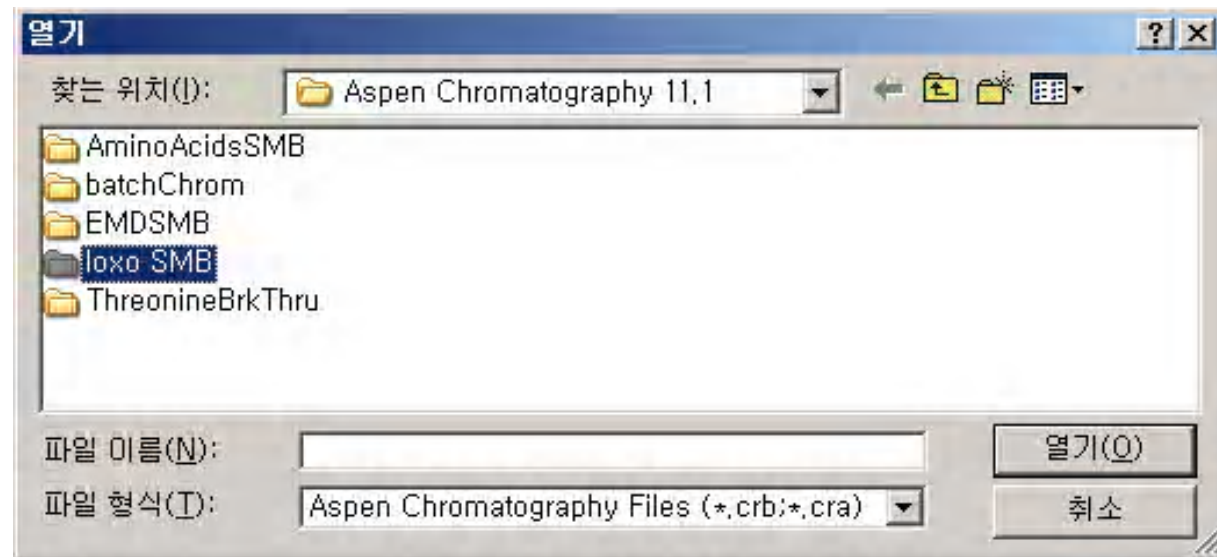


Fig. Picture of open menu

Aspen Chromatography - Ioxo SMB.cra

File Edit View Tools Flowsheet Run Window Help

Dynamic

Exploring

- All Items
 - Simulation
 - Flowsheet
 - Chromatography
 - SystemLibrary
 - Component Lists

Contents of Simulation

- Chromat...
- Component Lists
- Flowsheet
- Globals
- Open Library
- Solver Options
- SystemLi...

Process Flowsheet Window

Grid 0.05

Injection part →

Outlet part →

Column part →

Simulation Messages

Starting new snapshot file.
Simulation ready for solution
2 equations were not eliminated because they had residuals over 1e-007
A total of 419 equations (7.8%) were eliminated
Simulation has 6022 variables, 4972 equations and 19493 non-zeros

Ready Ready local Dynamic at 0 of 600

시작 Microsoft PowerPoint... Aspen Chromatog... 제목 없음 - 그림판

KO A 漢 오후 3:25

Configure Block/Stream TMB

Forms Variables Copy Print Help

Internal Columns

Adsorbent assumption: Fixed (SMB)

Recycle assumption: Closed Recycle

Number of columns in unit: 6 (2 to 40 only)

Port Position & Distribution

External Stream	Initial Port	Current Port
S1 - In	1	5
S2 - In	4	2
S3 - Out	2	6
S4 - Out	6	4

Port switching interval: 26.098 min

Recycle flowrate: 1.27704 ml/min

Specify Help **Click here**

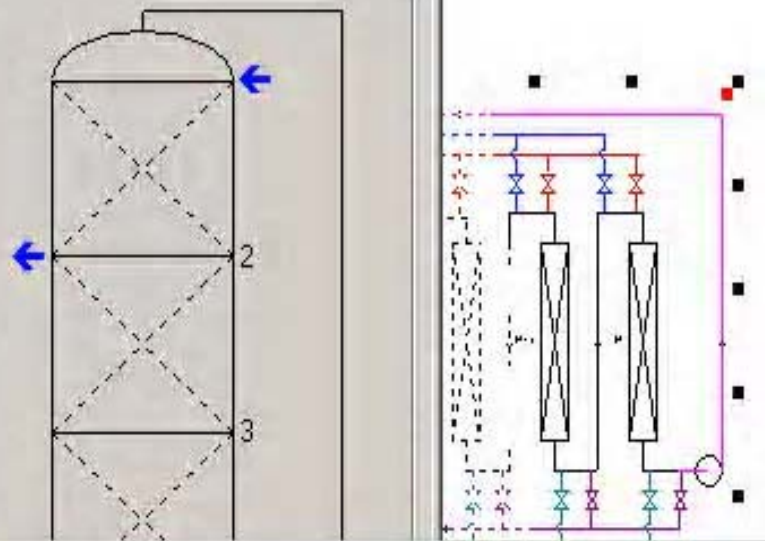
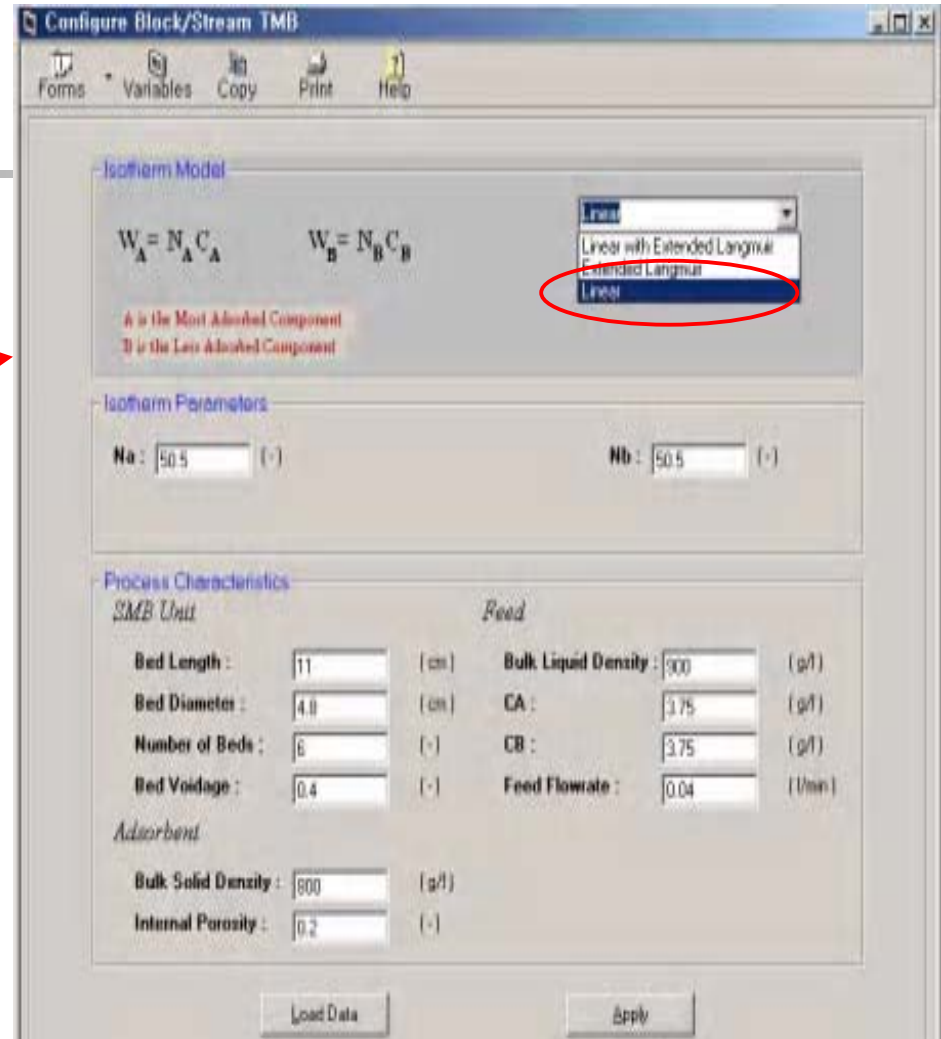
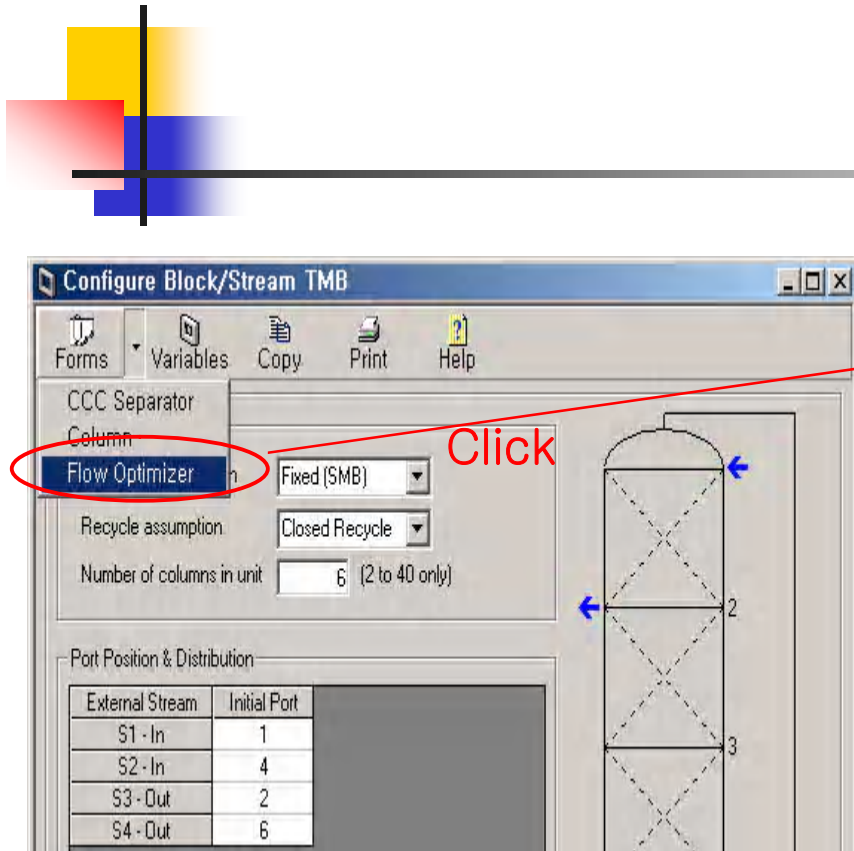
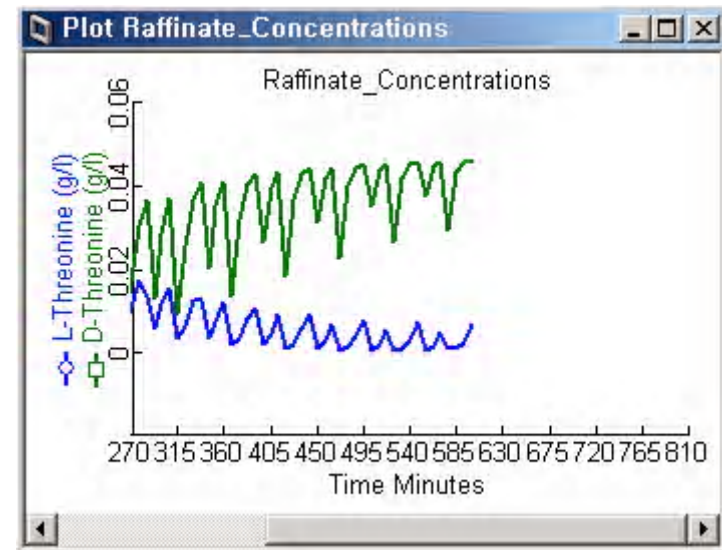
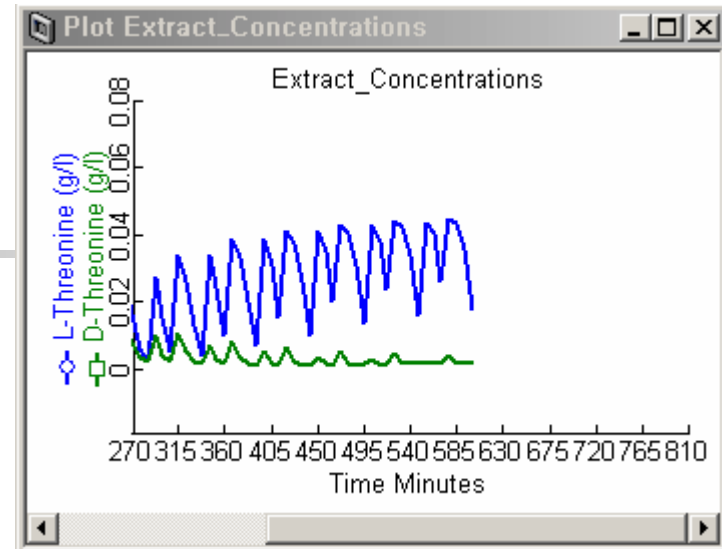
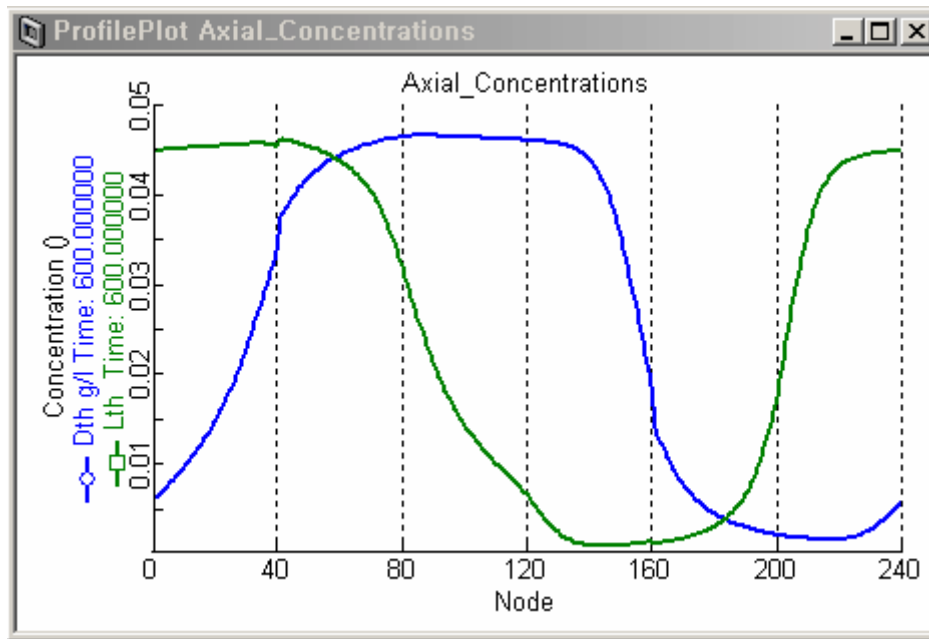
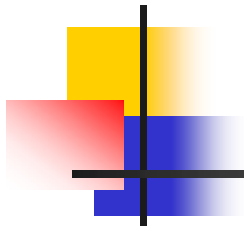
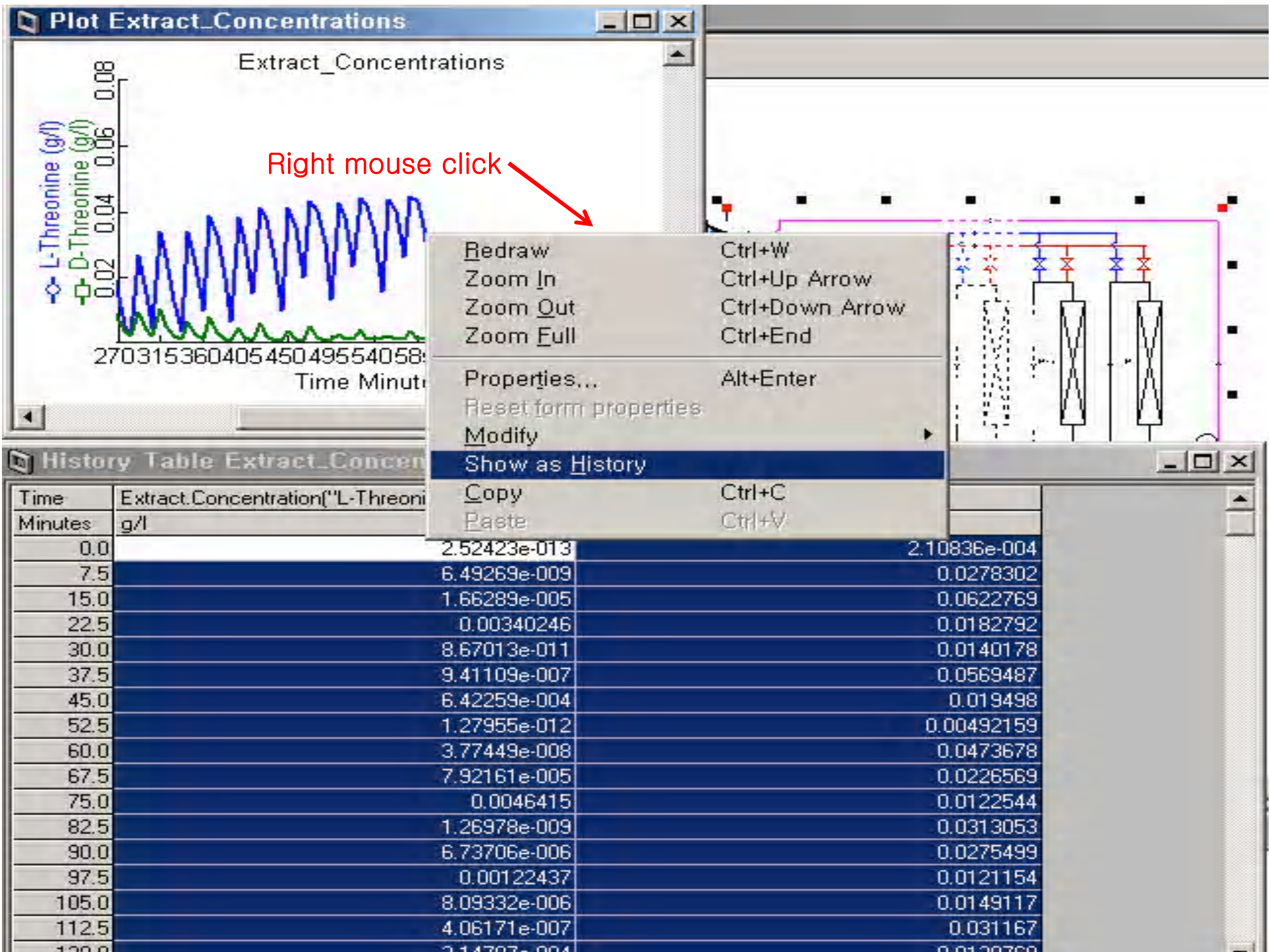


Table TMB.Specify

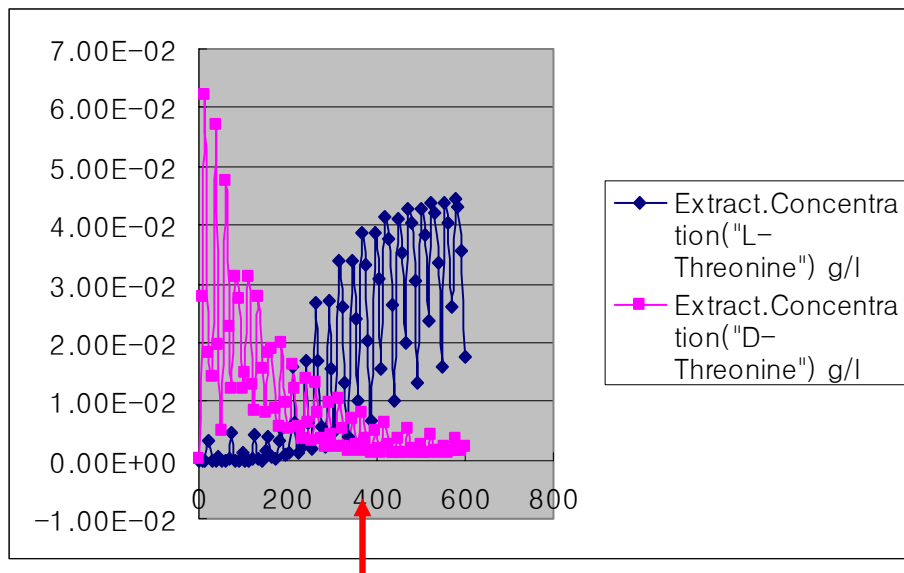
	Value	Spec	Units	Description
Hb	10.0	Fixed	cm	Height of adsor
Db	1.0	Fixed	cm	Internal diamete
Ei	0.53	Fixed	m3 void/m3 bed	Inter-particle voi
Ep	0.0	Fixed	m3 void/m3 bed	Intra-particle voi
Rp	5.0	Fixed	micron	Particle radius o
SFac	1.0	Fixed	n/a	Adsorbent sha
RHOI	996.0	Fixed	kg/m3	Mole density of
MUI	0.2	Fixed	cP	Liquid (Solvent)
MTC(*)				
MTC("D-Threoni	400000.0	Fixed	1/min	Constant mass
MTC("L-Threoni	400000.0	Fixed	1/min	Constant mass
IP(*)				
IP(1,"D-Threoni	7.901	Fixed	n/a	Isotherm param
IP(1,"L-Threoni	10.071	Fixed	n/a	Isotherm param



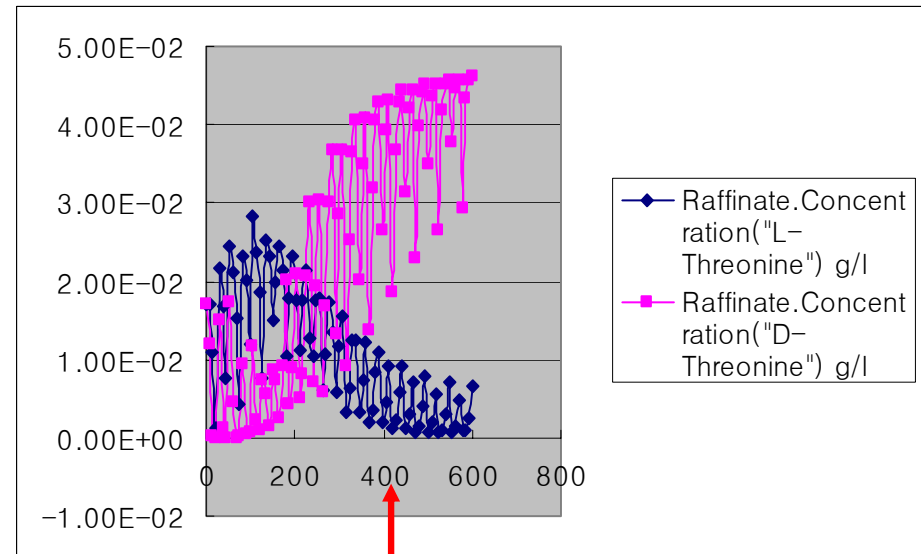




Results



◆ Extract concentrations



◆ Raffinate concentrations

MTC(mass transfer coefficient) change

Aspen Chromatography - Ioxo SMB.cra

File View Tools Run Window Help

Dynamic

Configure Block/Stream TMB

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Specify

Type: chrom_ccc_separator2

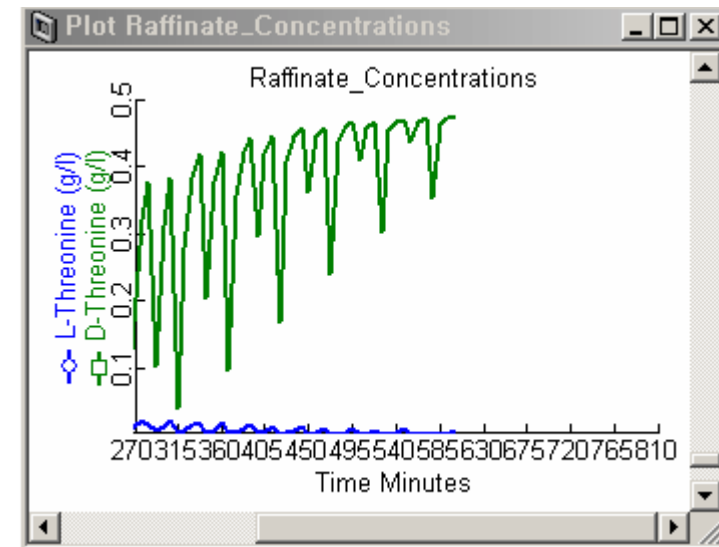
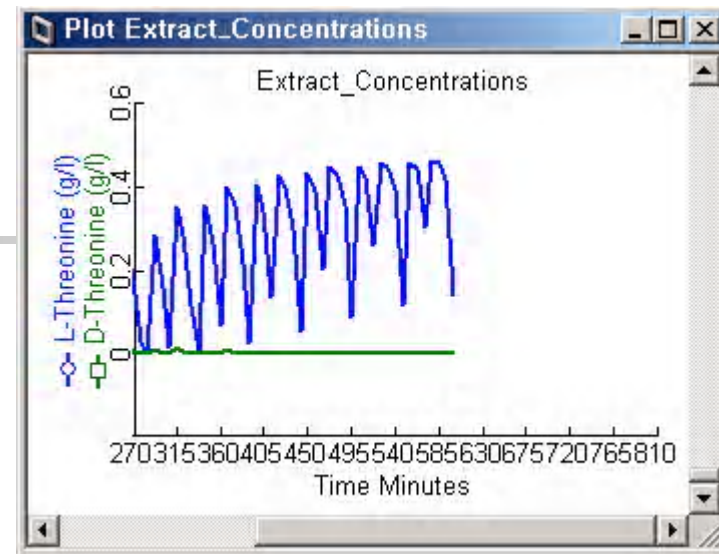
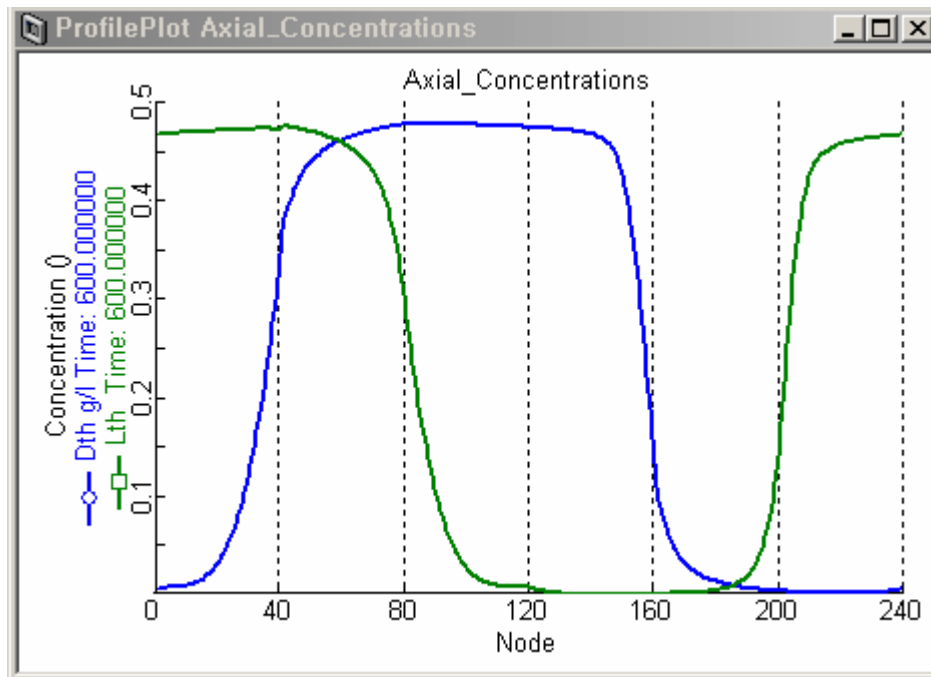
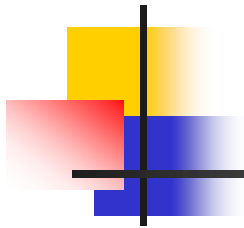
Table TMB.Specify

	Value	Spec	Units	Description
Hb	10.0	Fixed	cm	Height of adsorbent layer
Db	1.0	Fixed	cm	Internal diameter of adsorbent layer
Ei	0.53	Fixed	m ³ void/m ³ bed	Inter-particle voidage
Ep	0.0	Fixed	m ³ void/m ³ bed	Intra-particle voidage
Rp	5.0	Fixed	micron	Particle radius of adsorbent
SFac	1.0	Fixed	n/a	Adsorbent shape factor
RHOI	996.0	Fixed	kg/m ³	Mole density of eluent
MUI	0.2	Fixed	cP	Liquid (Solvent) viscosity
MTC(*)				
MTC("D-Threonine")	400000.0	Fixed	1/min	Constant mass transfer coefficient
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IP(*)				
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IP(2,"D-Threonine")	0.0	Fixed	n/a	Isotherm parameter

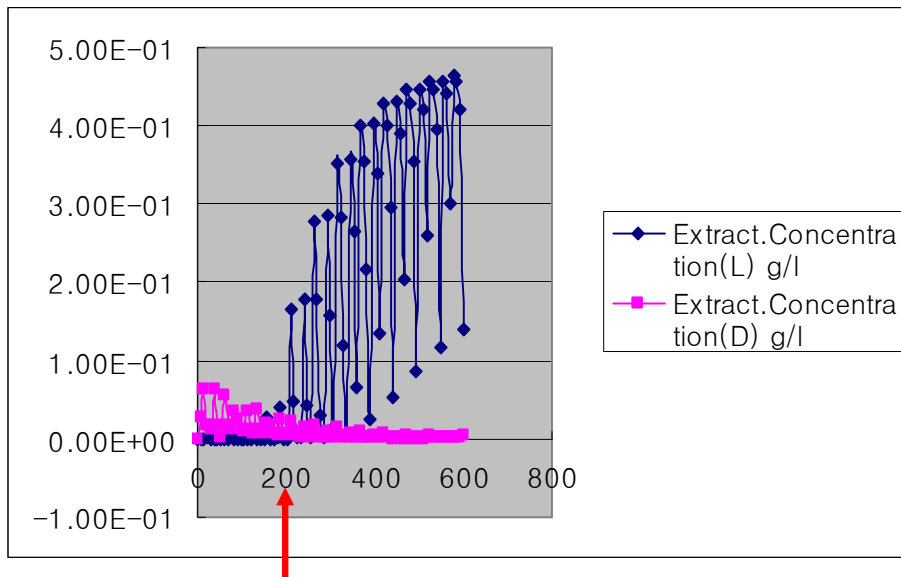
Click here

MTC(mass transfer coefficient) change

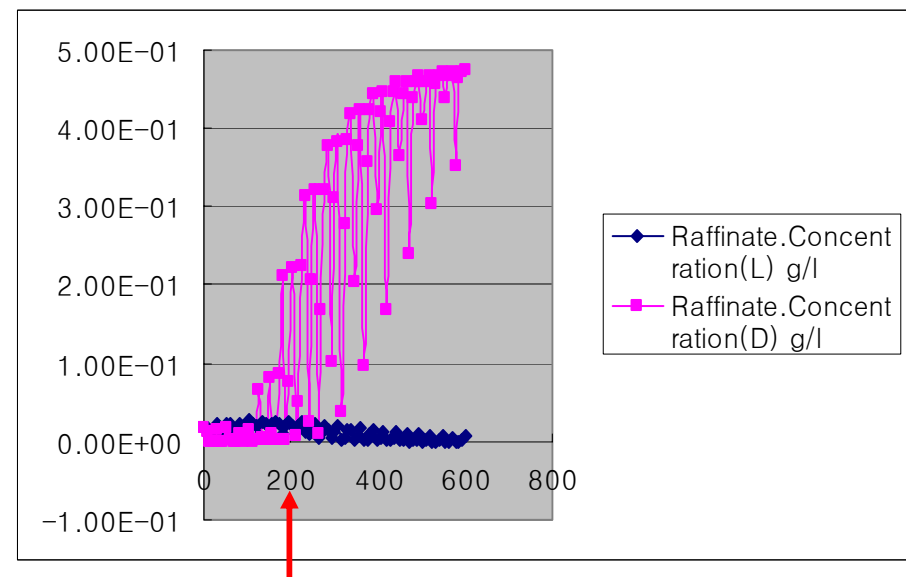
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Ep	0.0	Fixed	m3 void/m3 bed	Intra-particle voidage
Rp	5.0	Fixed	micron	Particle radius of adsorbent
SFac	1.0	Fixed	n/a	Adsorbent shape factor
RHOI	996.0	Fixed	kg/m3	Mole density of eluent
MUI	0.2	Fixed	cP	Liquid (Solvent) viscosity
MTC(*)				
MTC("D-Threonine")	20000.0	Fixed	1/min	Constant mass transfer coefficient
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IP(1,"D-Threonine")	7.901	Fixed	n/a	Isotherm parameter
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Results



◆ Extract concentrations



◆ Raffinate concentrations



Summary

- MTC change
- Transient ime (400min→200min)
- Aspen SMB simulation : Prerequisite before
SMB experiments