SMB Simulation Using ASPEN Chromatography

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1. Isotherm Calculation

- Isotherm of ketoprofen racemate

$$\bar{C}_R = 10.25 C_R$$

$$\bar{C}_S = 8.44 C_S$$

  - Assumption
    - ✓ Linear concentration range
    - ✓ Non-competitive adsorption-desorption process

Pulse injection

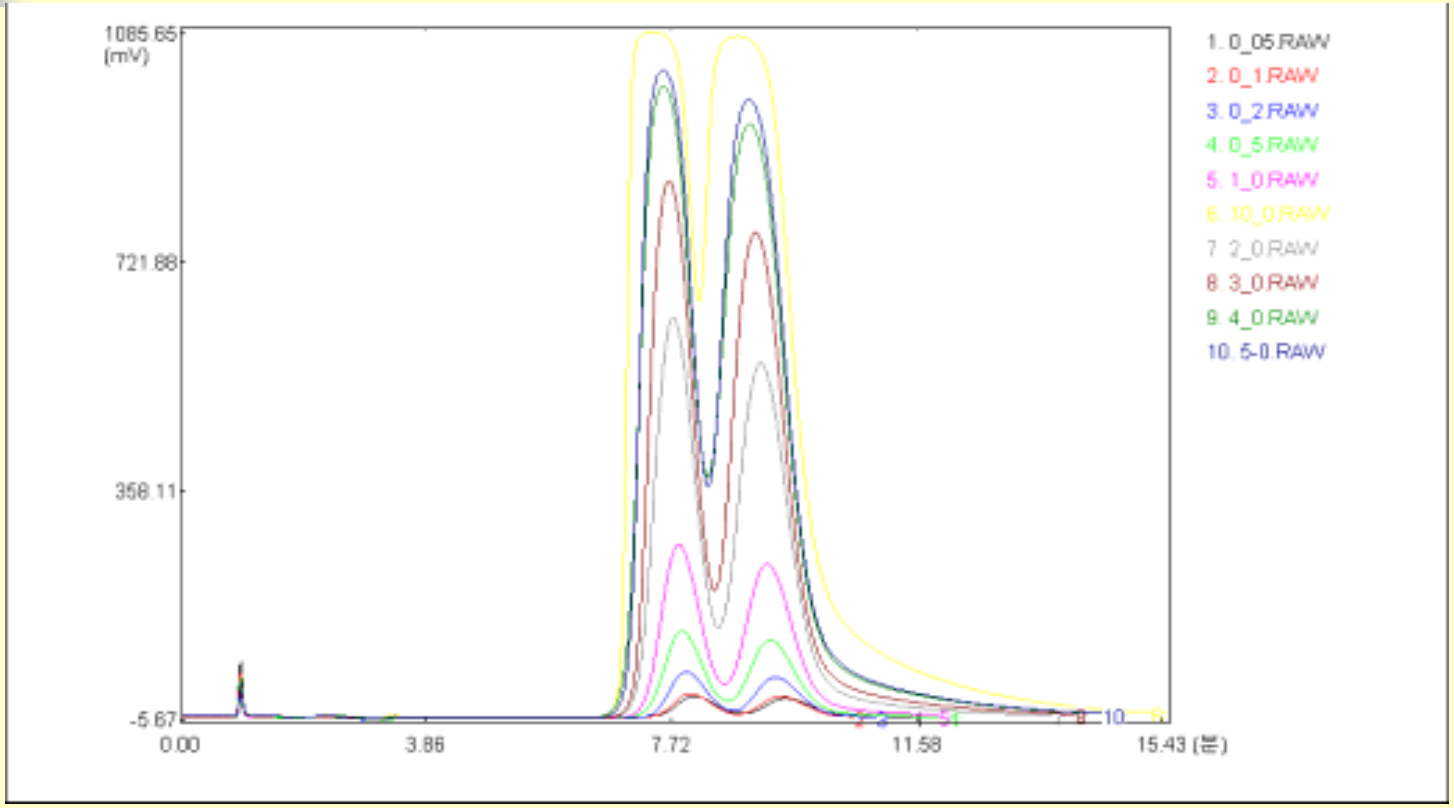


Fig. Pulse injection experiments at different concentrations; sample volume=100$\mu\ell$, wavelength=254nm, column=10cmx1cm

Table. Retention times measured from the different concentrations of samples; concentration of analytical feed was 0.025mg/ml, retention times used calculation were ½ retention times between start and maximum of peak heights.

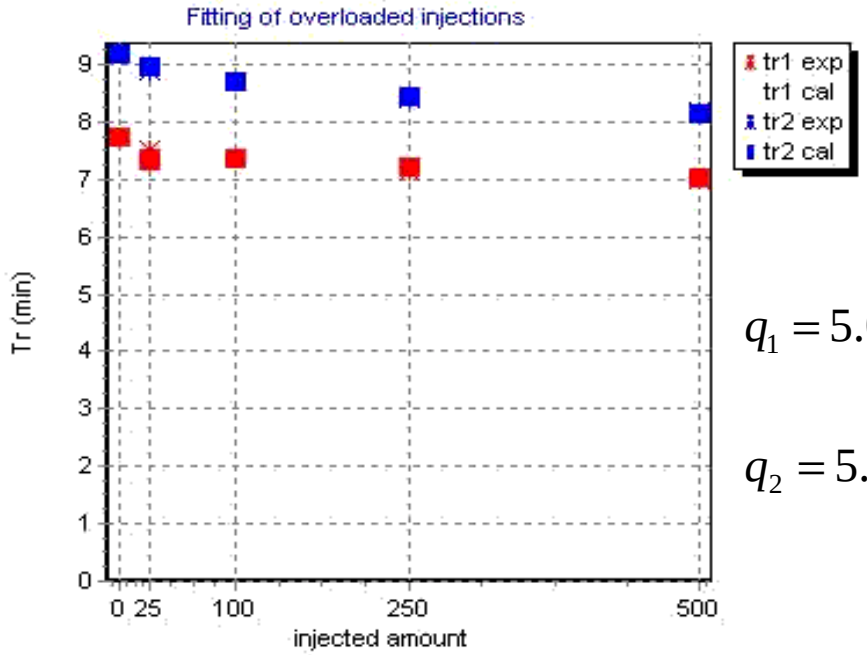
Overloaded injections

	Q (mL/min)	Vinj (uL)	C1 (g/L)	C2 (g/L)	tr1 (min)	tr2 (min)
inj 1	4.73	100	0.25	0.25	7.53	8.88
inj 2	4.73	100	1.0	1.0	7.36	8.69
inj 3	4.73	100	2.5	2.5	7.13	8.40
inj 4	4.73	100	5.0	5.0	7.00	8.2
inj 5						
inj 6						

Isotherms parameters

$$\overline{C}_i = \lambda . C_i + \frac{\overline{N}\widetilde{K}_i C_i}{1 + \widetilde{K}_1 C_1 + \widetilde{K}_2 C_2}$$

	λ	$\overline{N}\widetilde{K}i$	$\overline{N}$
Esp1	5.0	2.0922	4
Esp2	5.0	3.5577	4



Calculated Isotherm by PIM

$$q_1 = 5.0C_1 + \frac{2.0922C_1}{1 + 0.5231C_1 + 0.8894C_2} \text{ (Raffinate)}$$

$$q_2 = 5.0C_2 + \frac{3.5577C_2}{1 + 0.5231C_1 + 0.8894C_2} \text{ (Extract)}$$

Fig. Calculated isotherm parameters from HELP and modified competitive Langmuir isotherms of each ketoprofen enantiomer; retention times used calculation were ½ retention time of maximum peak height.

Fixed variables

Table . Specifications for SMB chromatography simulation

Specifications	Value
Column no.	6
Column diameter	1cm
Column length	10cm
Porosity	0.53
Mass transfer coefficient	1000/s
Diffusivity	$2*10^{5}$
Feed concentration	1mg/ml

Optimization flow rate of SMB with assumed isotherm

Optimum point in triangle area

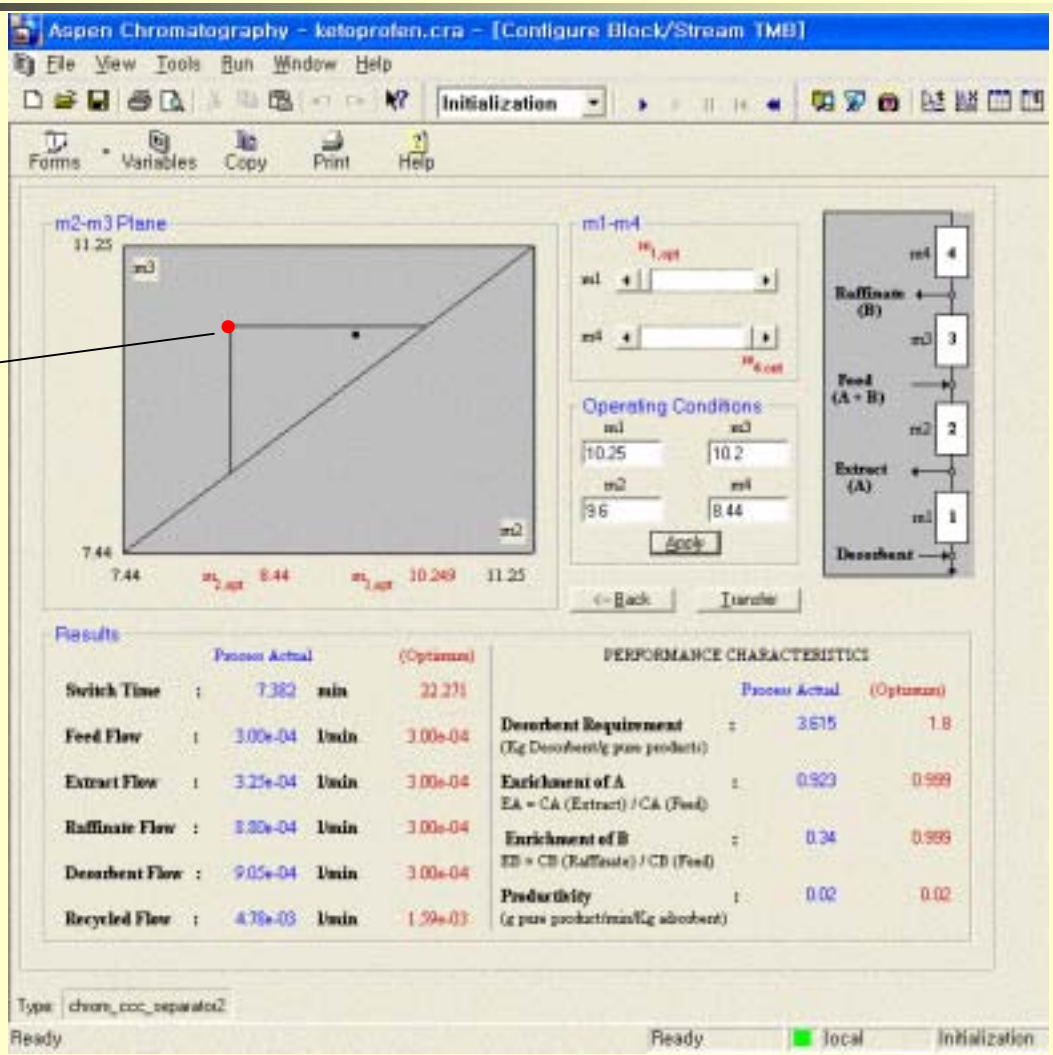
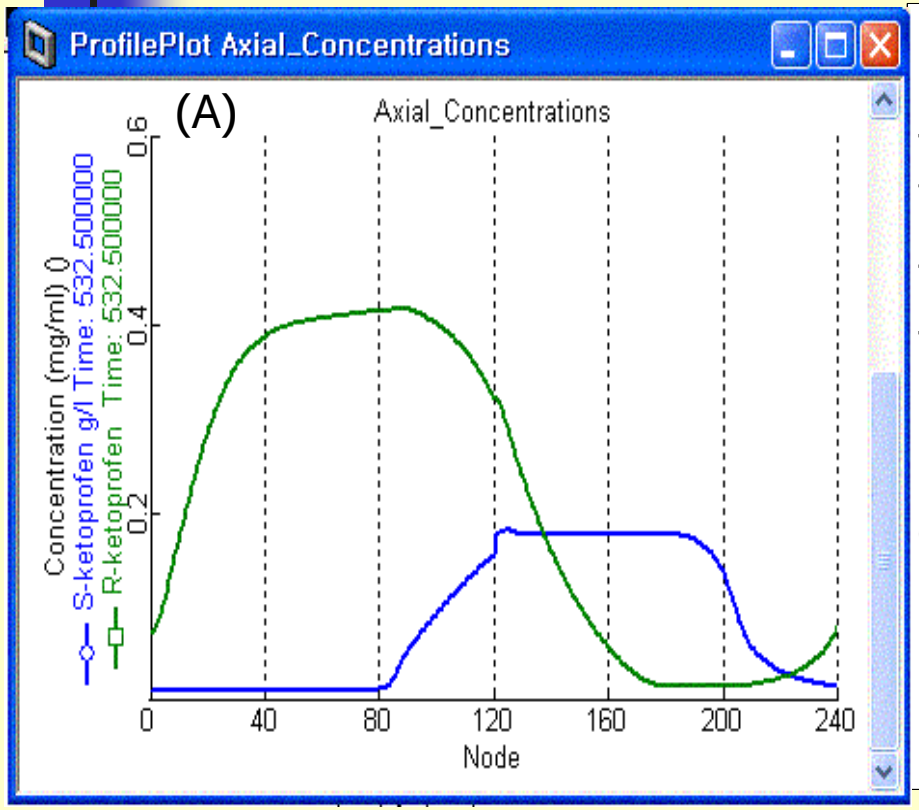


Fig. Optimization menu in ASPEN chromatography; m_2=9.6, m_3=10.2

Simulation results



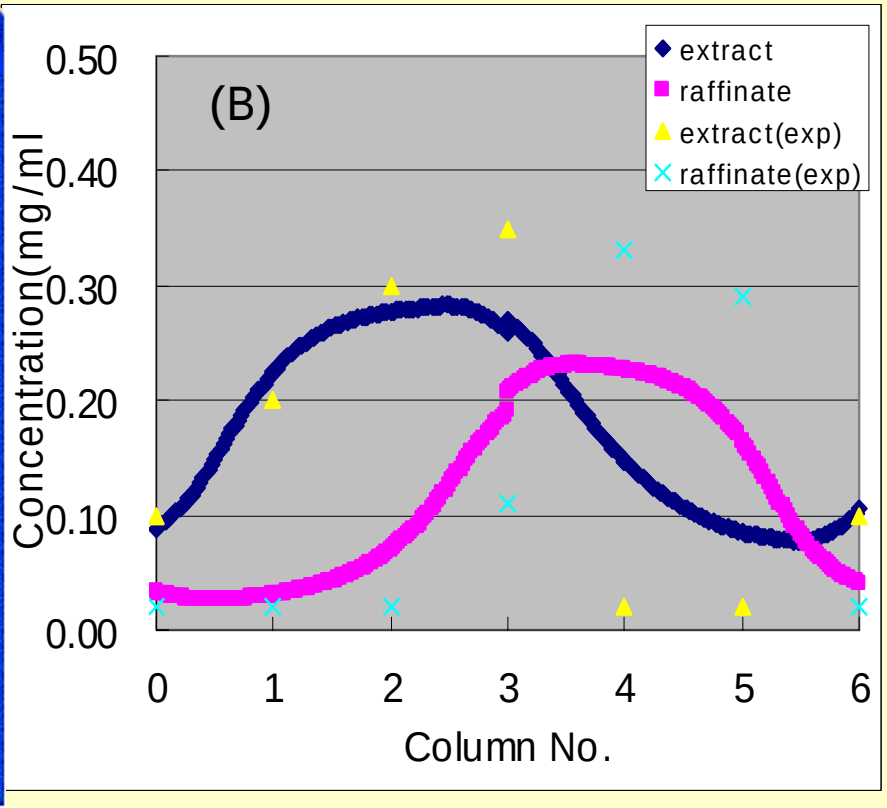


Fig. Comparison of simulation of internal concentration profile;(A): ASPEN (B): FORTRAN ;m2=9.6,m3=10.2

Simulation result

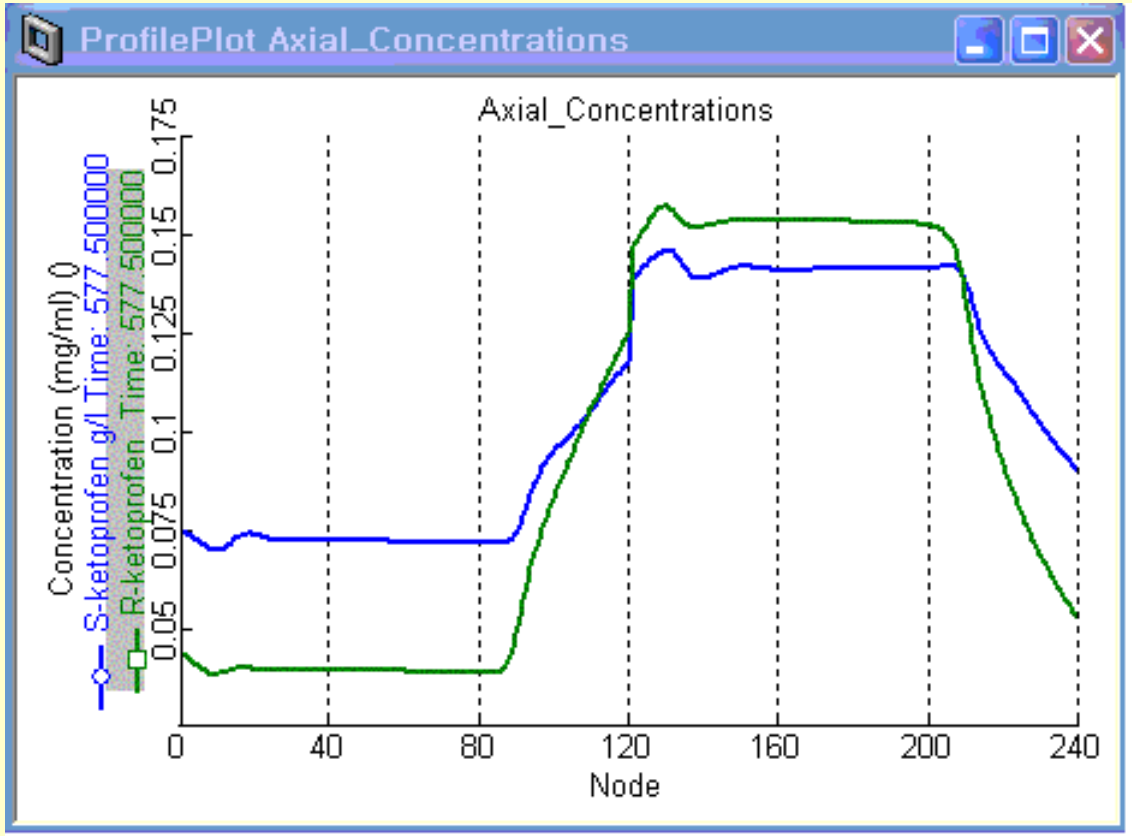


Fig. Simulation results of the same flow rates conditions at the previous case using calculated competitive Langmuir isotherms.

Optimization flow rate of SMB with calculated isotherm

Optimum point in triangle area

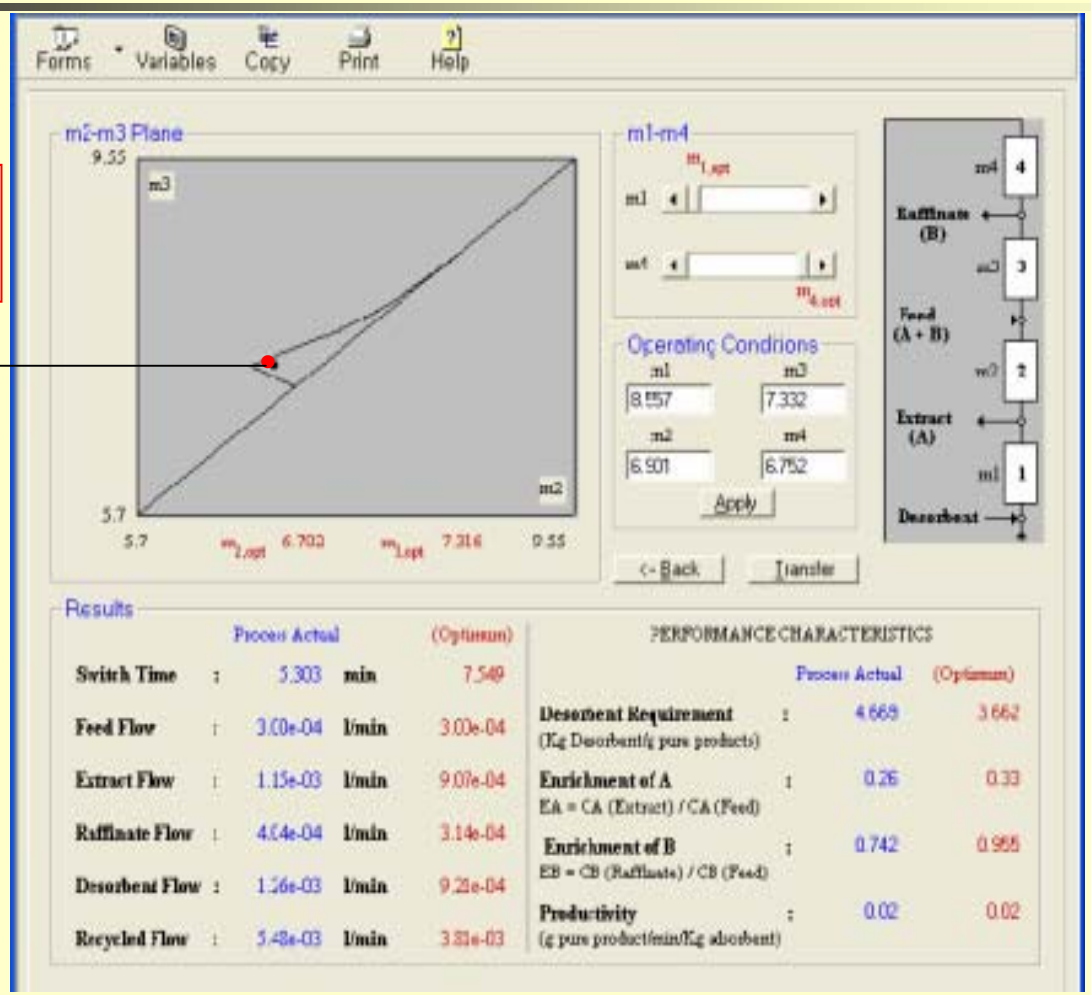


Fig. Optimization menu in ASPEN chromatography with calculated isotherm.

Simulation result

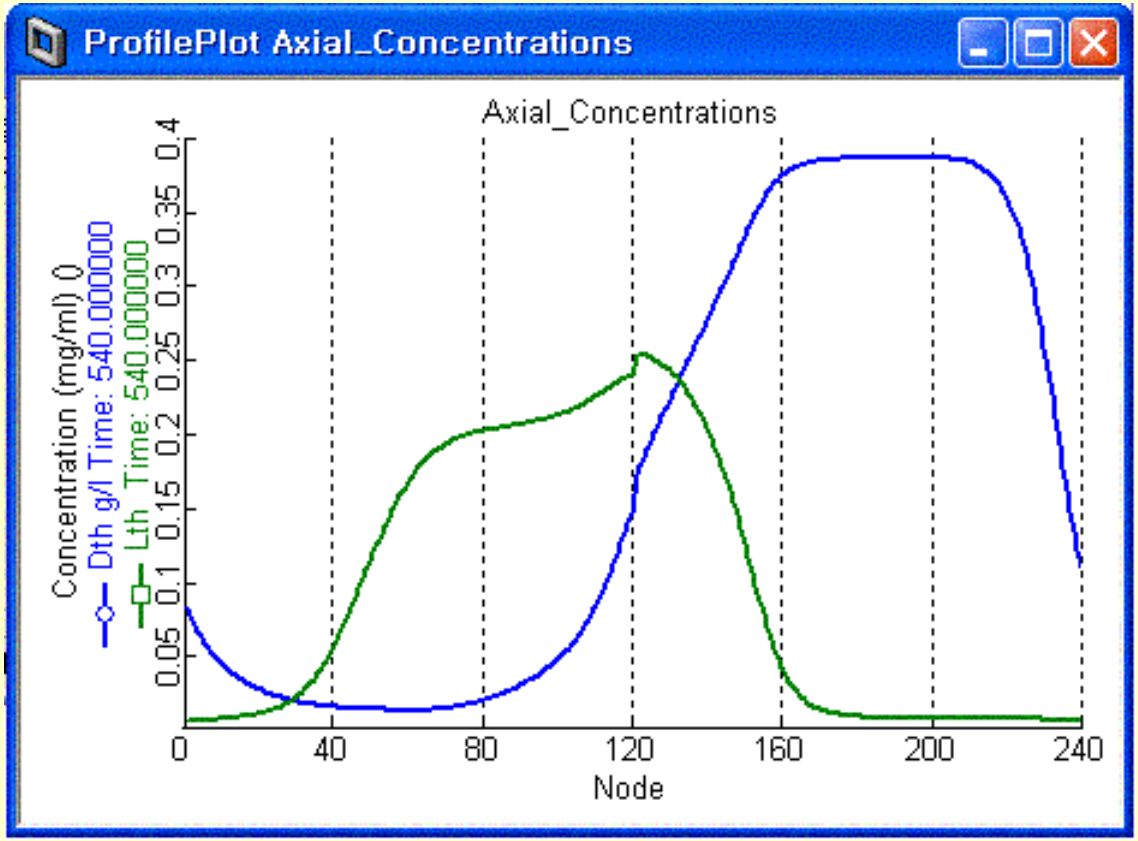
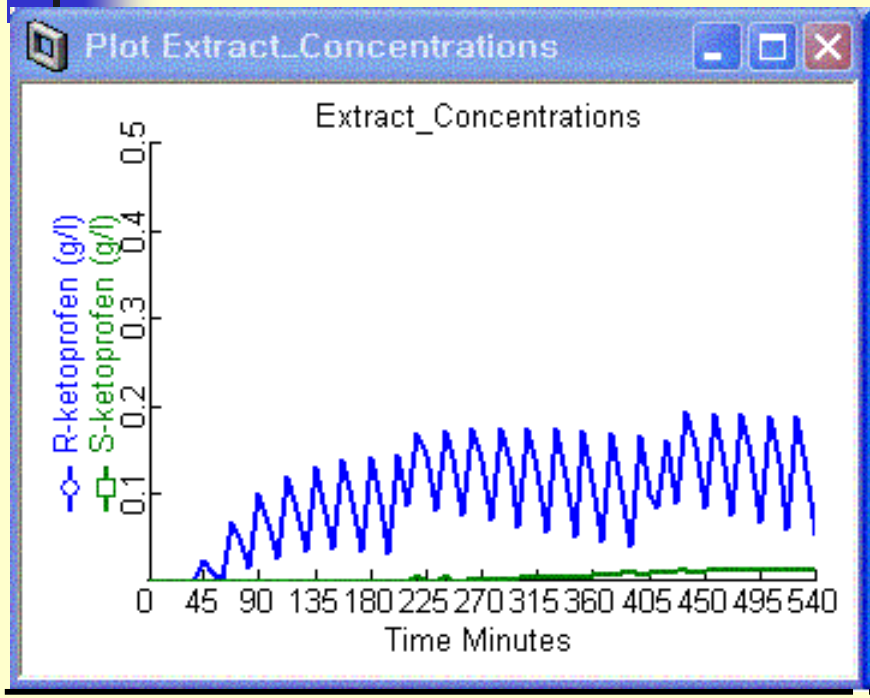
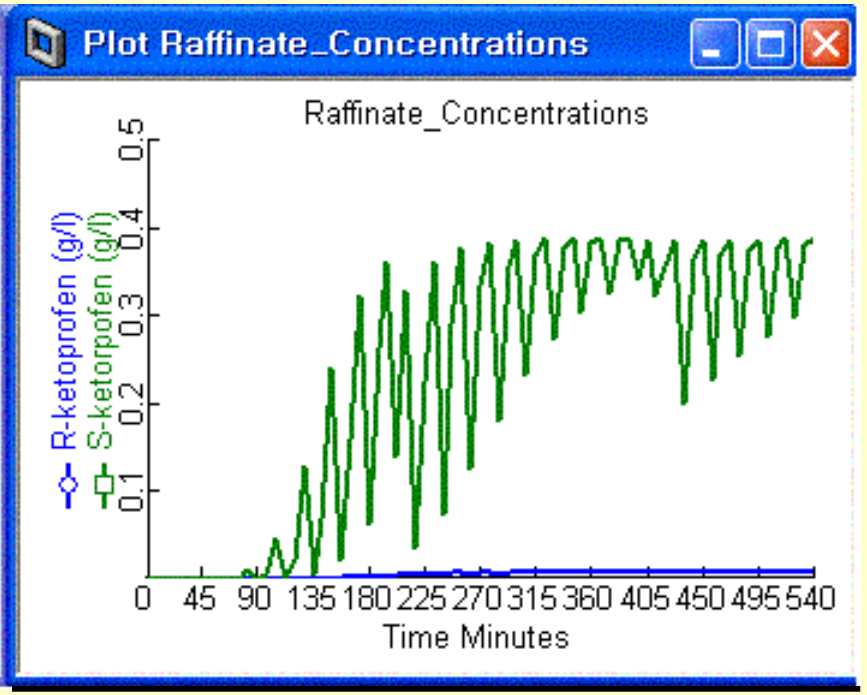


Fig. Simulation result provided from near point of optimum point using calculated competitive Langmuir isotherm.

Results





Concentration	Calculated value
S-ketoprofen	0.02 (G/L)
R-ketoprofen	0.05 (G/L)
Total concentration	0.7 (G/L)
Purity of S-ketoprofen	22.5 (%)
Purity of R-ketoprofen	77.5 (%)

Concentration	Calculated value
S-ketoprofen	0.39 (G/L)
R-ketoprofen	0.01 (G/L)
Total concentration	0.39 (G/L)
Purity of S-ketoprofen	97.9 (%)
Purity of R-ketoprofen	2.1 (%)

Concluding remark

- Aspen chromatography was good utility for estimation of SMB operation parameters
- But, it demands the exact isotherms calculated from other methods
- Additive experiments have to be perform with the results calculated from ASPEN simulator.