

Simulated Chromatography Data

Chromatographic System Constants:

Column Length	$L := 0.25 \cdot \text{m}$
Column Holdup Time:	$t_m := 1.00 \cdot \text{min}$

Sample Retention Information:

Capacity factor for compound a	$k_a := 0.65$
Capacity factor for compound b	$k_b := 0.95$
Number of theoretical plates	$N := 4000$

Sample Quantitation:

	Compound #1	Compound #2
Relative Response	$RR_a := 9.81695$	$RR_b := 9.1387$
Sample Concentration	$C_a := 20.341$	$C_b := 41.003$

Calculations:

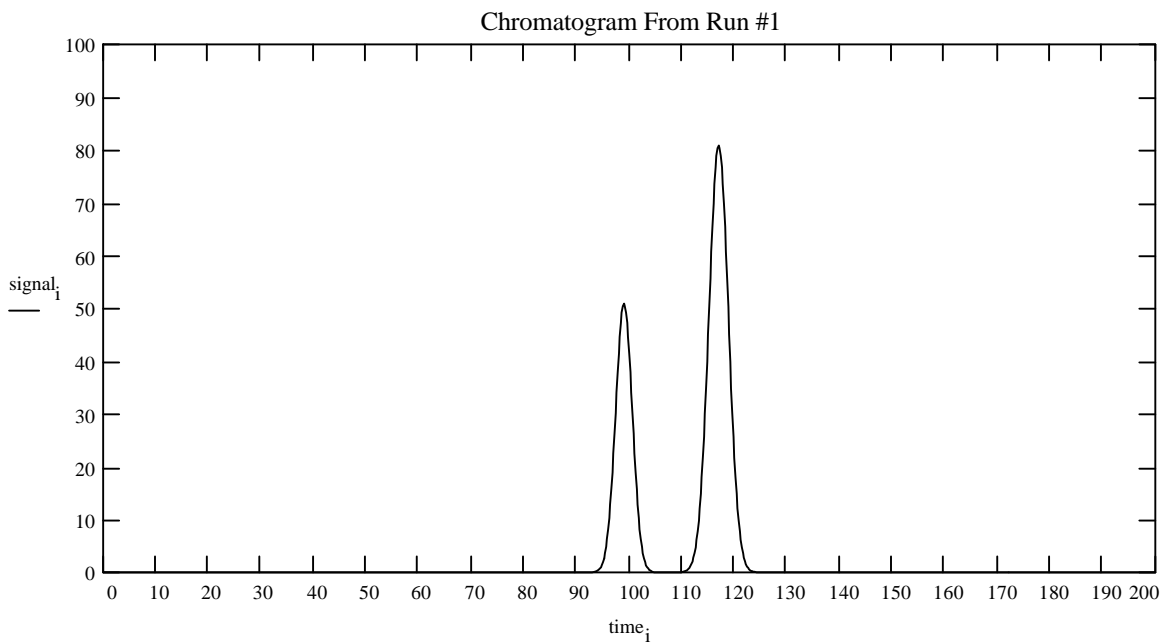
Retention Time	$t_a := k_a \cdot t_m + t_m$	$t_b := (k_b) \cdot t_m + t_m$
Peak Width	$\sigma_a := \frac{1}{\sqrt{N}} \cdot t_a$	$\sigma_b := \frac{1}{\sqrt{N}} \cdot t_b$
Width at half height	$W_a := \sqrt{5.54} \cdot \sigma_a$	$W_b := \sqrt{5.54} \cdot \sigma_b$
Relative Retention	$\alpha := \frac{k_a}{k_b}$	
Resolution	$R := \frac{ t_b - t_a }{0.5 \cdot (W_a + W_b)}$	
Counting Index	$i := 0, 1.. 1000$	$\text{time}_i := (0 + (i \cdot 0.2)) \cdot \text{sec}$

Chromatogram

$$\text{signal}_{a_i} := C_a \cdot \text{RR}_a \cdot \left[\left(\frac{1 \cdot \text{sec}}{\sigma_a \cdot \sqrt{2 \cdot \pi}} \right) \cdot e^{-\frac{1}{2} \cdot \left(\frac{\text{time}_i - t_a}{\sigma_a} \right)^2} \right]$$

$$\text{signal}_{b_i} := C_b \cdot \text{RR}_b \cdot \left[\left(\frac{1 \cdot \text{sec}}{\sigma_b \cdot \sqrt{2 \cdot \pi}} \right) \cdot e^{-\frac{1}{2} \cdot \left(\frac{\text{time}_i - t_b}{\sigma_b} \right)^2} \right]$$

$$\text{signal}_i := \text{signal}_{a_i} + \text{signal}_{b_i}$$



Calculated Parameters

	Compound a	Compound b
Retention Time	$t_a = 99 \cdot \text{sec}$	$t_b = 117 \cdot \text{sec}$
Peak Width (+/- 1 σ)	$\sigma_a = 1.565 \cdot \text{sec}$	$\sigma_b = 1.85 \cdot \text{sec}$
Peak Width (FWHM)	$W_a = 3.684 \cdot \text{sec}$	$W_b = 4.354 \cdot \text{sec}$
Peak Height	$\max(\text{signal}_a) = 50.892$	$\max(\text{signal}_b) = 80.808$
Peak Area	$\sum(\text{signal}_a) = 998.433$	$\sum(\text{signal}_b) = 1.874 \cdot 10^3$
Relative Retention	$\alpha = 0.684$	
Resolution	$R = 4.478$	

Questions.

1. Change the column length. What effect does this have on the chromatogram? What effect does this have on the calculated parameters?
2. Change the number of theoretical plates. What effect does this have on the chromatogram? What effect does this have on the calculated parameters?
3. Change the capacity factors for both compounds. What effect does this have on the chromatogram? What effect does this have on the calculated parameters?
4. Now that you have found a way to control the resolution. What resolution is required to distinguish the two peaks? What happens if one peak is much larger than the other? What tradeoffs are involved in the resolution?

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