PC simulation of analysis of n-alkanes by gas chromatography

Target of the simulation practice is to determine n-alkane in the sample. Prior to the analysis it is necessary to optimise separation conditions according to resolution (R), elution (capacity) factor (k), and time of analysis.

Task 1. Important parameters for gas chromatografic analysis

Find and write parameters of your chromatographic system using simulation programme GCSIM (Column, Temp, Detec) and discuss their influence on separation of n-alkanes in your sample

Column	
Column length	
Capillary	
Film thickness	
Carrier gas	
Pressure	
Temperature program	
Begin temperature	
Isothermal period	
End temperature	
Gradient	
Detection	
Injection volume	

Task 2. Comparison of separation on capillary and packed column

A: Compare chromatograms of n-alkanes C_6-C_{13} on capillary and packed column using isocratic elution at 150 °C (Change all temperatures for isocratic elution: **Temperature, Begin, Plateau** and **End** to 150°C). Find parameters of n-alkanes of our interest (tR -**Sample**, R-resolution v **Modl**-). To change the column type press **Column Type Packed**. If there are not all of analysed substances eluted in pre-set time, change time of analysis. (**Detect, Interval**, the first digit is active, e.g. 2 for 21 minutes, etc.)

	Capillary column		Packed column	
	tR/min	R	tR/min	R
Hexane				
Heptane				
Octane				
Nonane				
Decane				
Undecane				
Dodecane				
Tridecane				

B: Change **inject volume** from 1 µl to 100µl. What change in chromatogram can you observe? What column is more suitable for n-alkanes analysis? Why?