Selskabet for Analytisk Kemi

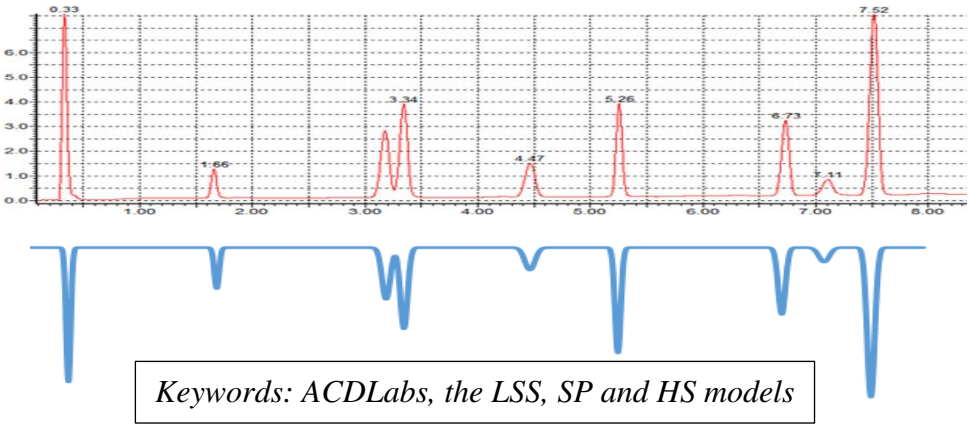
analytiskkemi.dk

København, den 12. februar 2021

Møde i SAK mandag den 8. marts 2021 på Zoom kl. 16.00-18.00

Meeting in SAK Monday March 8 2021 on Zoom at 4.00 - 6.00 PM

Prediction/simulation of chromatography



Keywords: ACDLabs, the LSS, SP and HS models

16:00 Patrik Petersson, Principal Scientist, Novo Nordisk A/S:
Practical approach to retention modelling to facilitate development of analytical chromatography methods: Advantages, principles, and possible pitfalls

16:50 Bo Svensmark, Assoc.Prof. Emeritus, Analytical Chemistry, PLEN, KU:
Digital simulation of GC and HPLC

17:20 Nikoline Juul Nielsen, Assoc. Prof., Analytical Chemistry, PLEN KU:
Using chromatographic simulations for teaching

17:35 Simon Stevns Larsen, Chemical Division, Danish Emergency Management Agency:
Linear solvent strength model in method development for the forensic analysis of Explosives by LC-MS

Bo Svensmark is inviting you to a scheduled Zoom meeting.
Topic: SAK meeting on Estimation and Simulation of Chromatography
Time: Mar 8, 2021 03:30 PM Paris
Join Zoom Meeting
https://ucph-ku.zoom.us/j/61961477633?pwd=cjdIVjJWSzBTUGVsLzBDZkxHSHB2UT09

Meeting ID: 619 6147 7633
Passcode: 006568

Everybody interested in analytical chemistry is welcome to attend the meeting. Zoom will be open from 3.30 PM

Practical approach to retention modelling to facilitate development of analytical chromatography methods: Advantages, principles, and possible pitfalls

Patrik Petersson
Principal Scientist, Novo Nordisk A/S

Principles and best practices for obtaining precise retention and resolution predictions to facilitate the optimisation of analytical chromatography will be discussed. How to generate accurate input data, the selection of appropriate models, and peak tracking will be addressed along with a suggested workflow. Adhesion to a few basic rules and simple precautions and the use of modern retention modelling software can assist the rapid development of robust and optimised analytical LC separation methods.

Digital simulation of GC and HPLC

Bo Svensmark
Assoc.Prof. Emeritus, Analytical Chemistry, ECP
Dept. of Plant and Environmental Sciences, University of Copenhagen

Simple software in Excel and Fortran for digital simulation of chromatography based on the Plate Theory using the Linear Solvent Strength model and Abrahams Solvation Parameter model will be presented. Input for the predictions are either experimental isocratic or isotherm retention factors or table values for columns and analytes for the Solvation Parameter model from literature. The results are prediction of chromatograms for gradient elution in HPLC and temperature programmed GC for any gradient or program you like. It will be shown that extension to nonlinear relations between retention factors and elution strength in HPLC and temperature in GC greatly improves the prediction accuracy.

Using chromatographic simulations for teaching

Nikoline Juul Nielsen
Assoc.Prof., Ph.D., Analytical Chemistry, ECP
Dept. of Plant and Environmental Sciences, University of Copenhagen

Teaching examples of how to use simulation of chromatographic behavior to understand experimental results. A) Students determine Linear Solvent Strength model parameters experimentally for a set of analytes, and based on these parameters they simulate simulate gradient behavior. Subsequently they experimentally validate their simulated gradient chromatogram and further optimize speed and resolution in the lab. B) Students experimentally determine Hydrophobic Subtraction model column parameters for their RP column, and subsequently compares the column selectivity towards other types of RP columns. C) Students use simulations based on the Solvation Parameter model to understand selectivity of stationary phases in GC.

Linear solvent strength model in method development for the forensic analysis of Explosives by LC-MS

Simon Stevns Larsen
Chemical Division, Danish Emergency Management Agency

The linear solvent strength model was applied in the development of a LC-MS analysis for the identification of explosives.
The linear solvent strength model was in this work extended to include a temperature dependency and instead of experimental isocratic runs a series of gradient runs were used to predict the LSS parameters.
Digital screening of combinations of column, flow rate, temperature, gradient time and gradient elution window was carried out to find the optimal chromatographic conditions, which was then experimentally tested.

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One tap mobile
+4532713157,,61961477633#,,,,*006568# Denmark
+4589883788,,61961477633#,,,,*006568# Denmark

Everybody interested in analytical chemistry is welcome to attend the meeting!
Become a member of SAK: go to chemsoc.dk
Zoom will be available from 3.30 PM

Alle interesserede er velkomne til at deltage!
Bliv medlem af SAK via: chemsoc.dk
Zoom åbner kl. 15.30, så vi kan få teknikken på plads inden kl. 16.00