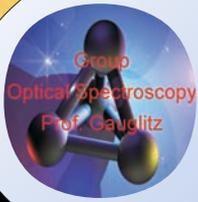


# Simultaneous Quantification of Mixtures of VOCs by Dynamic Single Sensor Set-ups: "Swiss Cheese like" Sensor Coatings for Size-Selective Discriminations

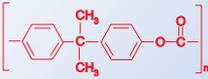


F. Dieterle, C. Betsch, S. Busche, G. Belge, B. Kieser, M. Harbeck, G. Gaudlitz

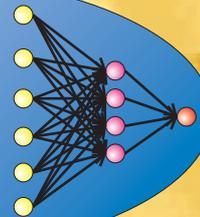
Institute of Physical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany

<http://barolo.ipc.uni-tuebingen.de>

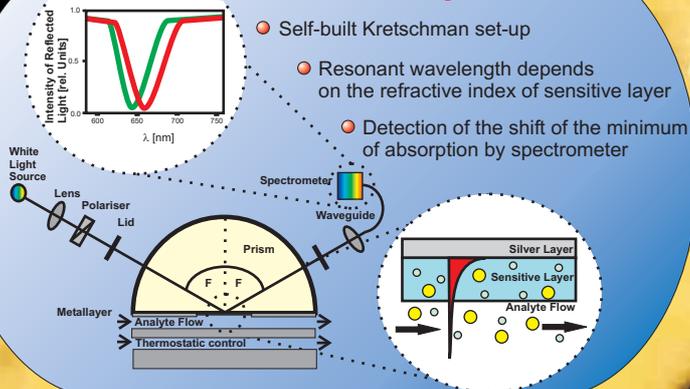
## A Microporous Polymer for Time-Resolved Measurements



- Makrolon is a commercially available polycarbonate with micropores of volumes of  $0.1 \text{ nm}^3$
- Different analytes show different sorption and desorption kinetics depending on the size of the analytes
- The sensor responses at different points of time during sorption and desorption are used as "virtual sensor array"
- In contrast to conventional sensor arrays, this "virtual sensor array" allows the parallel quantification of several analytes in mixtures by the use of only one "real sensor" with one sensitive layer
- The sensor responses of the different points of time are used as input variables for the data analysis by neural nets. The neural nets are trained with calibration data and predict subsequently the concentrations of independent test data

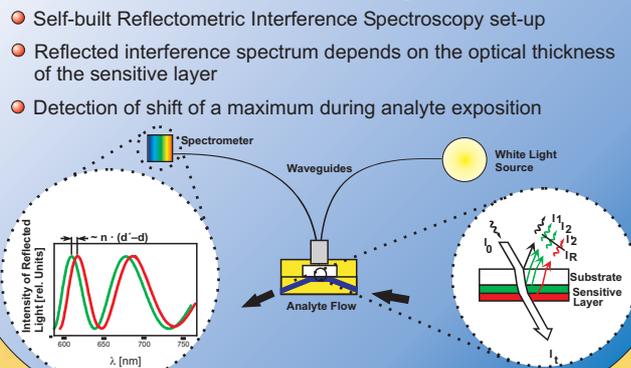


### SPR Set-up



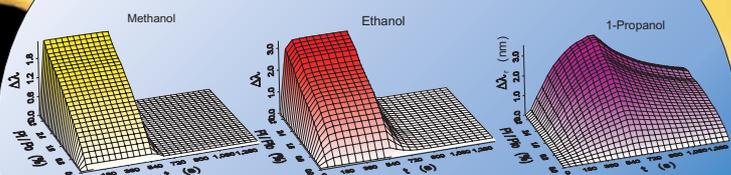
- Self-built Kretschman set-up
- Resonant wavelength depends on the refractive index of sensitive layer
- Detection of the shift of the minimum of absorption by spectrometer

### RfIs Set-up



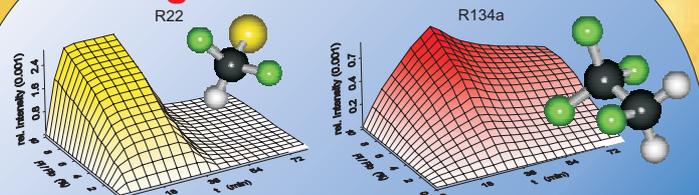
- Self-built Reflectometric Interference Spectroscopy set-up
- Reflected interference spectrum depends on the optical thickness of the sensitive layer
- Detection of shift of a maximum during analyte exposition

### Methanol, Ethanol, Propanol



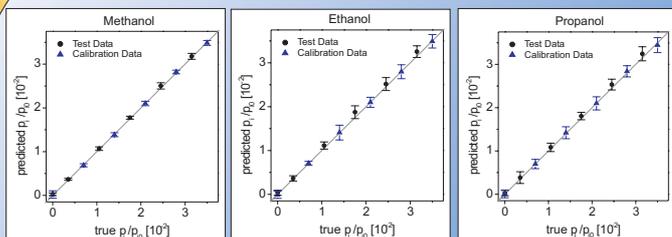
- The sorption and desorption kinetics of all three pure analytes differ depending on the size of the molecules
- As the time-concentration-response surface is different for all three analytes, a quantification in mixtures should be possible by the use of a non-linear multivariate data analysis (neural networks)

### Refrigerants R22 and R134a



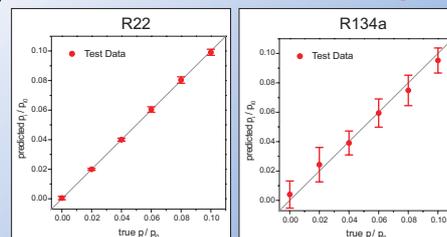
- The sorption and desorption kinetics of the smaller R22 is faster than the kinetics of the bigger R134a
- R22 belongs to the ozone depleting refrigerants and is gradually substituted by R134a in refrigerators and air-conditioners. An on-line quantification of R22 in mixtures of both refrigerants is needed

### Results for Ternary Mixtures



- Two full factorial designs for the calibration and test data. An accurate quantification with relative errors of 3.6 to 7.6 % was possible

### Results for Binary Mixtures



- The quantification of R22 in mixtures of R22 and R134a is very accurate with a relative RMSE of less than 3.3 %

- Full factorial designs of mixtures of both analytes were measured
- 420 predictions of test data were performed