

# **Direct measurement of diffusions coefficients in polymer solvent systems from spectroscopic data**

***David Siebel, Philip Scharfer, Wilhelm Schabel***

***Institute of Thermal Process Engineering, Thin Film Technology (TFT),  
Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany***

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Diffusion coefficients in polymer solvent systems are strongly dependent on the concentration of the solvent. Especially at low solvent concentrations the diffusion coefficients change by several orders of magnitude. Exact knowledge of the transport parameters is of crucial importance for the process design. In literature a large number of different measurement techniques has been discussed. All of them have specific advantages and disadvantages. Nevertheless, the availability of diffusion data in polymer solvent systems remains insufficient. Purely predictive methods, as the Free Volume Theory, have become increasingly complex but do not show satisfactory results.

In this work, a new concept for a fast and reliable determination of concentration-dependent diffusion coefficients in polymer solvent systems is discussed. The method promises to make diffusion data over a wide concentration range available with a single experiment. The diffusion coefficients are calculated directly from concentration gradients obtained from spectroscopic data. Measurement data is provided by means of inverse micro raman spectroscopy (IMRS) which allows the in-situ measurement of solvent concentration in polymer solutions with high spatial and time resolution. For this direct determination no information on the boundary conditions and exterior mass transfer is needed.

For the calculation of diffusion coefficients, the experimental conditions and the data processing routines have to be optimized. With a suitable method of smoothing, scattering of measurement data can be reduced. Furthermore, an approximation of the local mass flux, which cannot be measured directly, has to be found. Different

approaches to these challenges have been tested and the influence on the quality of the results has been evaluated. Initial results for relevant material systems are shown and discussed on the basis of existing data.