REVIEW OF THE DIPLOMA THESIS

Zdeněk Preisler: "Computer Modeling of Branched Polymers"

The scope of the Diploma Work is the modeling the conformation behaviour of the linear and branched polymers. Special attention is paid to the behaviour of the polymer molecules in the pores of the chromatographic packing, used in size-exclusion chromatography (SEC). The theme of the Thesis is interesting and important because SEC is one of the most important methods of polymer characterization and its mechanism is not known in all details. The author has contributed to the software modeling by implementing the self-avoiding mechanism into the molecular-dynamics modeling which is the prerequisite for the modeling of separation of real polymers.

The work is well organized and clearly written. The results are a contribution to molecular dynamics and give also insight into mechanism of chromatography of polymers.

The research was based on a well founded literary survey which gives information necessary to understand the molecular-dynamics, Monte Carlo and Self-Consistent field methods used.

It would be interesting to discuss the results of the work in the broader context of the SEC separation theory, i.e., of the relation between different radii and the product of intrinsic viscosity and molecular weight, which is generally considered the universal separation parameter in SEC, called hydrodynamic volume. In the text to Fig. 3.7, it is stated that "that calibration curve constructed using hydrodynamic radius is suitable for evaluation the elution behavior of randomly branched polymers." because all points fall on the same line. However, several authors, *e.g.*, Farmer *et al.*, infirm this criterion [*Int. J. Polym. Anal. Charact.*, 11 (2006) 3-19] showing that polymers with different degree of branching show different hydrodynamic radii at the same elution volume. Please, can you comment on this?

Some formal details were discussed with the author.

The thesis fulfills all requirements and is recommended for the defense.

Netolik (

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