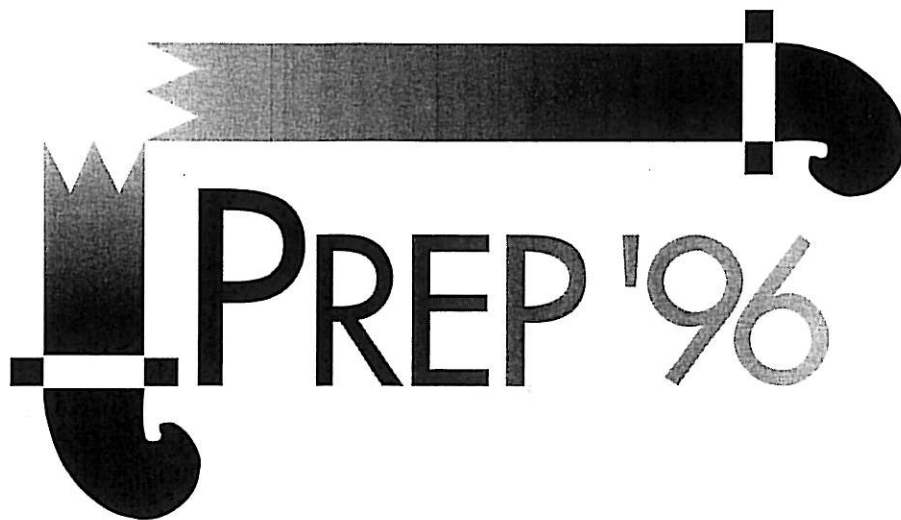


**Pais, L.S., Loureiro, J.M., and Rodrigues, A.E.**

Modeling, Simulation and Operation of a Simulated Moving Bed for Continuous Chromatographic Separation of 1,1'-bi-2-naphthol Enantiomers in *PREP'96 International Symposium on Preparative and Industrial Chromatography and Related Techniques*, Basel, Switzerland, September 1-4, 1996. (*comunicação oral*)



PREP '96

**FINAL PROGRAM**

INTERNATIONAL SYMPOSIUM  
ON PREPARATIVE AND  
INDUSTRIAL CHROMATOGRAPHY  
AND RELATED TECHNIQUES

SEPTEMBER 1 - 4, 1996

CONVENTION CENTER BASEL,  
BASEL, SWITZERLAND

UNDER THE AUSPICES OF  
NEW SWISS CHEMICAL SOCIETY  
SOCIÉTÉ FRANÇAISE DE CHIMIE  
GESELLSCHAFT DEUTSCHER CHEMIKER

## Innovative Processes including Electrochromatography

Chair:

Frank Volker Schurig, Universität Tübingen, D  
Klaus K. Unger, Universität Mainz, D

**08.45 – 09.00** Opening of the Symposium

Eric R. Francotte, Ciba, CH-Basel

**09.00 – 09.40** Advances in Preparative Separation Technologies –  
Do we need to advance Technology or Acceptance?

Invited Lecture: Reinhard Ditz, Merck KGaA, LPRO Chrom, D-Darmstadt

**09.40 – 10.05** Preparative Isoelectric Focusing in a Multi-  
Compartment Electrolyzer with Immobilized  
Membranes

Elisabeth Wenisch, Universität Wien, Institut für angewandte Mikrobiologie,  
A-Wien

**10.05 – 10.30** Large-Scale Protein Separation with the Gradiflow

Garry Corrhals\*, Keith Williams, Stephen Horvath, Andrew Gooley,  
Macquarie University, School of Biological Sciences, AUS-Sydney

10.30 – 11.00 Coffee Break

Chair: Roger-Marc Nicoud, NOVASEP, Vandoeuvre-lès-Nancy, F  
Michel Perrut, Separex, Champigneulle, F

**11.00 – 11.25** Preparative Supercritical Fluid Chromatography for  
the Production of Highly Concentrated  
Dodecaheptaeneacid-ethyl ester

Gerd Brunner\*, F. Reichmann,  
Technische Universität Hamburg-Harburg, D-Hamburg

**11.25 – 11.50** The Preparative Enantiomer Separation of the Chiral  
Inhalation Anesthetics Enflurane, Isoflurane and  
Desflurane by Gas Chromatography on a  
 $\gamma$ -Cyclodextrin Derivative

Frank Volker Schurig\*, Markus Juza, Heiko Grosenick, Universität Tübingen,  
Institut für Organische Chemie, D-Tübingen

**11.50 – 12.15** True-Moving-Bed Chromatography: Compact-  
Disc-HPLC (CD-HPLC) / New Stationary Phases

Andreas Kühn, Michael Kühn\*, CONCHROM Trenntechniken GmbH  
& Co. KG, D-Bremen

14.00 – 16.00 Poster Session

## Simulated Moving Bed Chromatography

Chair:

Geoffrey B. Cox, Prochrom, Champigneulle, F  
Andreas Seidel-Morgenstern,  
Otto-von-Guericke-Universität Magdeburg, D

**16.00 – 16.25** Optimal Operation of Simulated Moving Bed  
Units for Nonlinear Chromatographic Separations

Massimo Morbidelli\*, Marco Mazzotti, Maria Pia Pedferri,  
ETH Zürich, Chemical Engineering Department, CH-Zürich

**16.25 - 16.50** Continuous Chromatographic Techniques for  
Processing Multi-Component Feedstocks

L.J. Bauer\*, J.W. Priegnitz, A.K. Chandhok, S.A. Wilcher,  
UOP Inc., USA-Des Plaines, IL

**16.50 – 17.15** Large Scale Separation of Isomers by Simulated  
Moving Bed

Roger-Marc Nicoud\*, P. Adam, J. Bléhaut,  
NOVASEP SA, Chromatographie, F-Vandoeuvre-lès-Nancy

**17.15 – 17.40** Modeling, Simulation and Operation of a  
Simulated Moving Bed for Continuous  
Chromatographic Separation of  
1,1'-Bi-2-Naphthol Enantiomers

Alirio Rodrigues\*, Luis S. Pais, José M. Loureiro,  
Universidade do Porto, LSRE School of Engineering, P-Porto

18.00 – 19.00

Reception in the Foyer (2nd Floor)  
of the Convention Center Basel,  
offered by the Government of Basel-City

**MODELING, SIMULATION AND OPERATION OF A SMB FOR SEPARATION OF 1,1'-Bi-2-NAPHTHOL ENANTIOMERS**

L. Pais, J. Loureiro and A. Rodrigues\*  
LSRE School of Engineering  
Universidade do Porto  
Porto, Portugal

The objective of this paper is to study the separation of enantiomers of 1,1'-bi-naphthol in 3,5-dinitrobenzoyl phenylglyzine bonded to silica using heptane/isopropanol (72/28) as eluent by SMB chromatography.

A model for the prediction of the steady state performance of the SMB was developed assuming axial dispersion flow, LDF approximation for intraparticle mass transfer and multicomponent adsorption equilibria.

The SMB package allows the simulation of the pilot unit. The effect of switching time, extract and feed flowrates, section length and number of mass transfer units was analyzed. The performance was characterized by purity, recovery, productivity and solvent consumption. The package is an important tool for learning and training operators; it allows the choice of best operating conditions.

The operation of the SMB pilot unit was carried out for the separation of racemic mixtures using a 8 column configuration Purities as high as 94.5% of the more retained species in the extract and 98.9% of the less retained species in the raffinate were obtained.

The package was also used to predict the steady state internal profiles for the SMB operation in good agreement with experimental results.