# Numerical methods and applications in chemical distributed parameter systems (W. Schiesser and A. Vande Wouwer)

Alain Vande Wouwer
vdw@autom.fpms.ac.be
Faculte Polytechnique de Mons, Belgium

Partial differential equations (PDEs) arise in the mathematical description of a spectrum of chemical and physical applications, including chemical kinetics, heat and mass transfer, and fluid dynamics. The PDE models are usually highly nonlinear and therefore require numerical analysis and computer-based solution techniques.

Particular attention is paid in this minisymposium to the method of lines, a versatile computational approach to the solution of time-dependent PDEs, which basically proceeds in two separate steps:

(a) approximation of spatial derivatives using finite difference, finite element or finite volume methods

(b) time integration of the resulting system of semi-discrete initial-value equations using ODE or DAE solvers.

PDE models involving steep moving fronts (e.g. temperature or concentration fronts) generally require special care in their numerical solution, and space and time adaptation techniques, i.e. moving mesh or adaptive mesh refinement techniques, are currently of particular interest.

Besides numerical analysis and simulation of distributed parameter systems, other important issues, such as the estimation of unknown parameters in PDE models, the reconstruction of unmeasured variables using state observers (or software sensors), as well as process optimization and control, are addressed in this minisymposium, with emphasis on advanced numerical techniques and practical case studies.