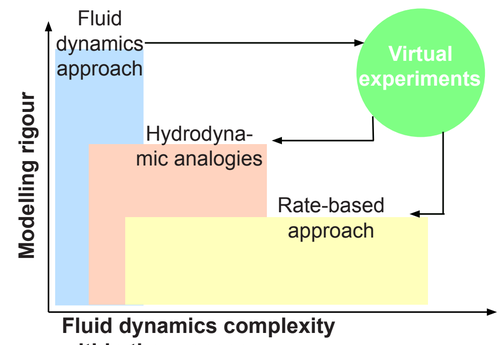
UNIVERSITÄT PADERBORN
Die Universität der Informationsgesellschaft

Complementary Modelling of Fluid Separation Processes

Principle

Despite that different fluid separations have much in common, a unified approach to their modelling is missing. This is mainly due to the diversity of operating, scale and boundary conditions as well as due to the significant modelling difficulties. A unified modelling approach is particularly difficult to formulate when a direct account of the process rates (transport and reaction kinetics) is essential, which is common in design and optimisation tasks. Therefore, we suggest an alternative way and present a novel modelling methodology which comprises different specific kinetics-based approaches and combine them in a complementary way. Such complementary modelling is a promising means to support the development of sustainable chemical engineering processes.



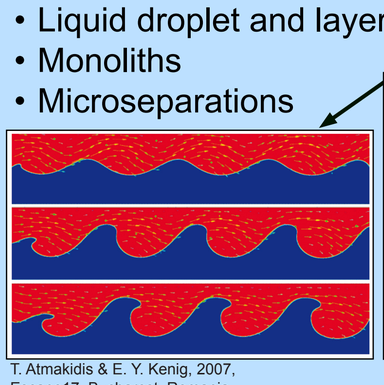
Main Results

Fluid-dynamics approach

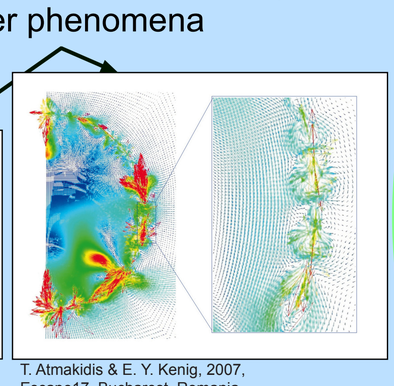
Idea: Process description by partial differential equations of fluid dynamics

Characteristics:
- Provides full information about the process (velocity,temperature
- and concentration field) in a purely theoretical way
- Difficult to apply for complex multiphase flow patterns

Results obtained:
- Fim flows (cocurrent and countercurrent, laminar and turbulent, binary and multicomponent, one-, two- and three-phase, non-reactive)
- Liquid droplet and layer phenomena
- Monoliths
- Microseparations



T. Atmakidis & E. Y. Kenig, 2007, Escape17, Bucharest, Romania



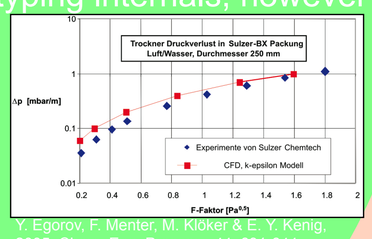
T. Atmakidis & E. Y. Kenig, 2007, Escape17, Bucharest, Romania

Virtual experiments

Idea: Replacement of empirical parameter estimation by model-based simulations for different basic types of column internals

Characteristics:
- Extracts information from the investigation of small periodic representative elements of real internals (usually via CFD)
- Provides a link between FDA and RBA/HA
- Potentially, a way to virtual prototyping internals, however still in the early stage

Results obtained:
- Pressure drop in fixed beds and structured packings →
- Residence time distribution in catalytic packings
- Gas-liquid mass transfer coefficients in catalytic packings
- Liquid-solid mass transfer coefficients in fixed catalyst beds



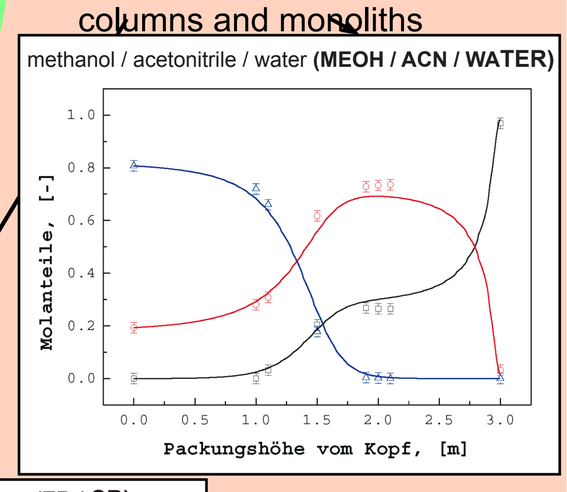
Y. Egorov, F. Menter, M. Klöker & E. Y. Kenig, 2005, Chem. Eng. Process., 44, 631-644

Hydrodynamic analogy approache

Idea: Development of analogies between real complex fna mics and geometrically simpler flow patterns based on experimental observations

Characteristics:
- Allows an extension of the application of partial differential equations to morecomplex objects and processes
- Model parameters are directly derived from the geometry of internals

Results obtained:
- Pertracton (liquid membrane ex-traction)
- Microdistillation
- Distillation in structured packed columns
- Reactive stripping in packed columns and monoliths

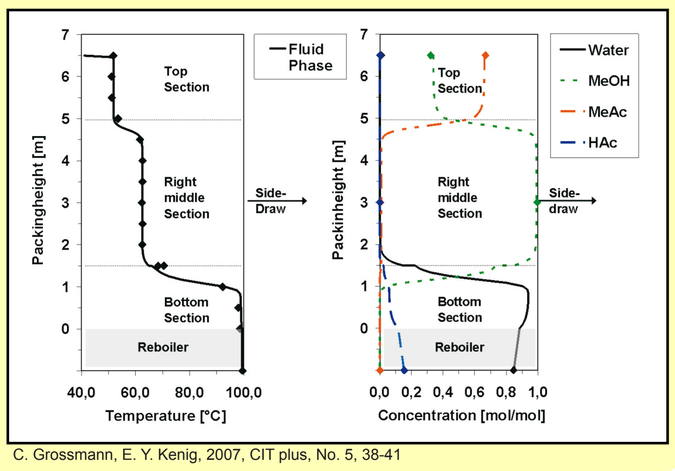


Fluid-dynamics approach

Idea: Column sub-division onto segments (stages) and their kinetics-based description

Characteristics:
- Suitable in design and optimisation tasks for many staged operations, including reactive and hybrid separations
- Weak point is that accuracy and predicti-vity strongly depend on the quality of mo-del parameters

Results obtained:
- Distillation and reactive distillation
- (Reactive) absorption and desorption
- Reactive Stripping
- Non-Reactive and reactive dividing wall columns
- Different Systems, units, internals
- Steady-state and dynamic simulations
- Optimisation studies



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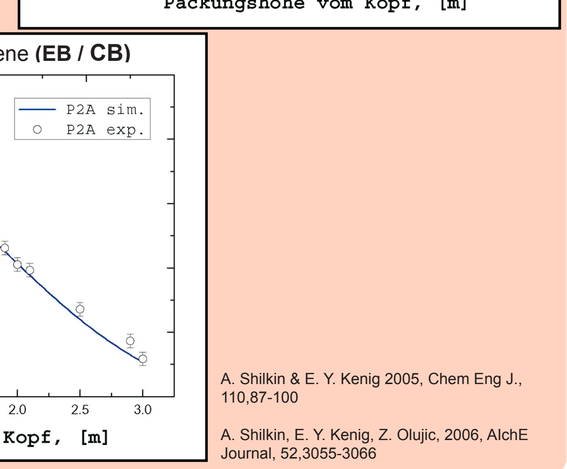


A. Shilkin & E. Y. Kenig 2005, Chem Eng J., 110,87-100

A. Shilkin, E. Y. Kenig, Z. Olujic, 2006, AIchE Journal, 52,3055-3066

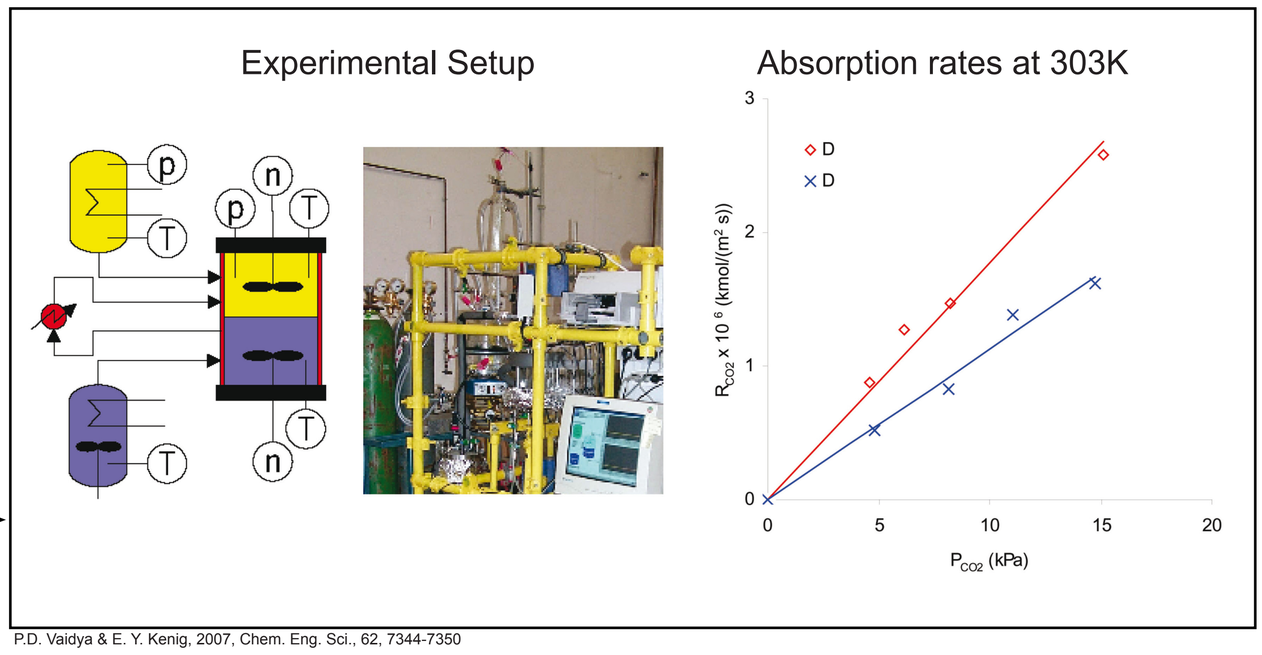
Extension

Idea: Reaction kinetics measurements for CO_2 absorption into aqueous blends of alkanolamines prepared from renewable resources

Characteristics:
- Data are obtained in a stirred cell reactor with a plane, horizontal gas-liquid interface
- Easy-to-use experimental device operated batch-wise
- The method is based on a simple fall-in-pressure technique,

  without measurements of concentrations

Results obtained:
- Absorption of CO2 into aqueous solutions containing N,N-diethylethanolamine (DEEA), N-ethylethanolamine (EEA) and their blends →
- Reaction acceleration by piperazine (PIP)



P.D. Vaidya & E. Y. Kenig, 2007, Chem. Eng. Sci., 62, 7344-7350

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