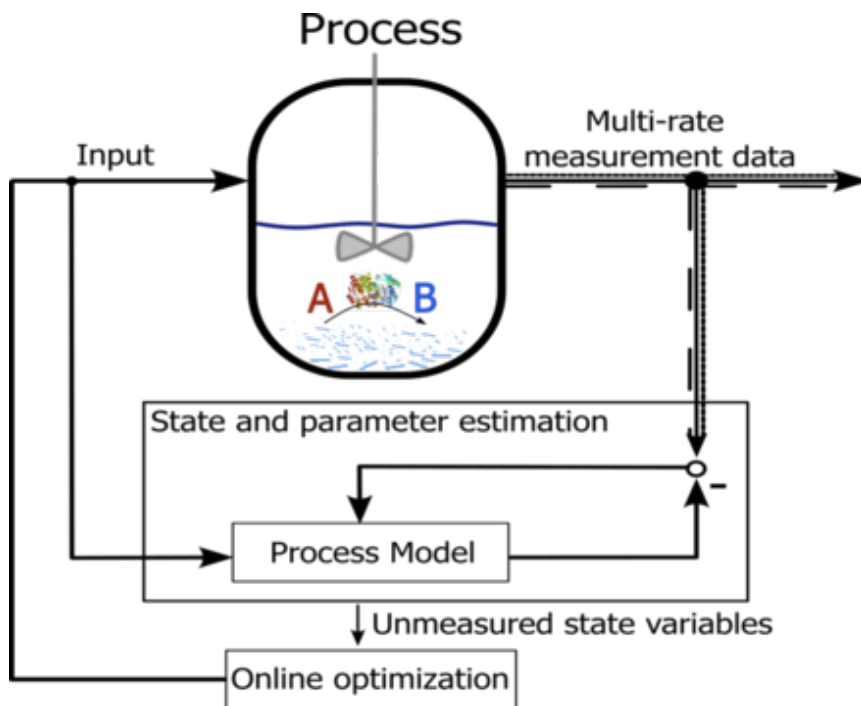


Subprogramme 7: Self-learning control of the catalytic conversion of olefins to α -amino acids and β -amino alcohols



The aim of this project is to develop self-learning control systems for the online optimization of the catalytic conversion of olefins to α -amino acids and β -amino alcohols.

The enzyme-catalyzed reactions of α -keto carboxylic acids to α -amino acids, in particular homophenylalanine, and α -hydroxyketones to β -amino alcohols, in particular homophenylalaninol, with integrated product crystallization will be considered as process examples. Subsequently, the membrane separation processes for catalyst and solvent separation will also be investigated.

For this purpose, a repetitive online optimization is carried out at 'single batch' and/or 'batch to batch' level, whereby the operating conditions are determined with the help of available measurement information and so-called hybrid mathematical models.

Hybrid modeling combines the basic knowledge of physical chemistry from the other subprojects with data-driven machine learning approaches. Essential work steps include: (i) the development of suitable hybrid models for the process steps under consideration, (ii) the development of suitable methods for the online adaptation of the developed models and (iii) efficient strategies for online optimization, (iv) the integration of the aforementioned methods within the framework of a self-learning control concept, (v) systematic *in silico* tests and (vi) finally, experimental validation in cooperation with the project partners.

The Team

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The Project

- ▶ Subprogramme 1: Homogeneous Catalysis
- ▶ Subprogramme 2: Oxidation Catalysis
- ▶ Subprogramme 3: Integrated Biocatalysis & Crystallization
- ▶ Subprogramme 4: Membrane Separation
- ▶ Subprogramme 5: In-Situ Analysis
- ▶ Subprogramme 6: Process Design
- ▶ Subprogramme 7: Process Control