

Title: EnzymeVision - Automated Kinetic Model Identification of Biocatalysts Under Process Conditions

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Description

The python scripts are used to automatically control four syringe pumps (AL-1000, World Precision Instruments, Saragosa, USA) to perform continuous experiments with a packed bed reactor with immobilized formate dehydrogenase. For monitoring, a flow through cuvette (170.700 QS, Hellma GmbH & Co. KG, Müllheim) is applied with a UV light source (DH-2000-BAL, Ocean Insight, Orlando, USA) and spectrometer (HR4000, Ocean Insight, Orlando, USA). The volume flow is monitored with a flow meter (SLF3S-0600F, Sensirion, Stäfa, Switzerland). The flow meter, spectrometer and daisy-chained syringe pumps are applied via USB to a Laptop.

Usage

To set experiments up with this software, initial experiments have to be specified with stock concentrations, inlet concentrations and residence times in UserInput.xlsx. Pump mode 3 specifies four syringe pumps with a defined diameter and volume. In Adminvalues.json, the COM ports for the devices and output path can be set. To start the experiments, the main_EnzymeVision_2022_06_22.py has to be started in e.g. Visual Studio Code with Python version 3.9.12. When the mail manager is used, an email address has to be set up and logged in with a password. After that, the experiments start automatically. In order to use the MATLAB script, the file have to be extracted in the Python script folder. In the MATLAB script (DesignOfExperiments), enzyme concentration, starting concentrations and residence times can be inserted. Furthermore, initial values, fitting tools and bound for model parameters can be changed.

Status of the project

The project is finished. And the python code is published first as version 1.0.

The description of the code and comprehensive results will be published in the dissertation "Automated Kinetic Model Identification of Biocatalysts Under Process Conditions" by Hennecke *et al.*

Some results will be published in "Closed-loop Identification of Enzyme Kinetics Applying Model-Based Design of Experiments" by Hennecke *et al.*

For optimal experimental designed experiments after the initial experiments, the MATLAB code by Lucas Schaare has to be applied. This will be published in the next version of this software package.

Thanks

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