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Identifying anaerobic digestion models using simultaneous batch experiments

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As in other wastewater treatment processes, anaerobic digestion models have become a valuable tool to increase the understanding of complex biodegradation processes, to teach and to communicate using a common language, to optimize design plants and operating strategies and for trying operators and process engineers. Models require accurate and significant parameter values for being useful. Although the calibration problem is an issue of concern, often is neglected. A method for calibration is the use of simultaneous batch experiments (SBE), which requires simple and usually available equipment, and is based on the analysis of replications and the responses obtained when starting from different initial conditions. The objective of the present work is to systematize the SBE method, illustrating and discussing the applicable steps.

The main steps of the method are: 1.) Set up the mathematical model and define the calibration problem. Namely, define exactly the problem to be solved; 2.) Preliminary experimental design approach. Set-up different SBE characterized by different initial conditions, define the output function, characterized by the variables that can be measured during the experiments, and define variables which initial values can be known; 3.) Perform a structural identifiability study, consisting of a theoretical analysis to find out whether the designed experiment can lead to a unique set of parameter values and unknown initial conditions (i.e., initial microorganisms concentrations); 4.) Perform the experimental design leading to parameters and initial biomass identification, based on previous step results; 5.) Perform the practical identification or estimation of the unknowns, as a result of optimizing an objective function, i.e. maximizing the sum of multiple determination coefficients for all measured variables and for all simultaneous experiments performed; 6.) Study the statistical characterization of estimated parameter values, calculating its confidence intervals, its statistical significance and the correlation matrix; and 7.) Return to step 4) or 1) if step 6) provides low significance levels for the calculated parameters or if the model structure cannot explain experimental behavior.

Taking into account that appropriate experimental design depends on kinetic parameters values, which determination is, actually, the objective of the work, results of previous experiments or results from literature are required to orientate initial substrate and biomass concentrations to be used, in order to obtain an experimental design allowing unique and significant parameter values. The explanation of every step is done providing the theoretical basis, discussing applicable methods and equations, and illustrating with examples, some of them previously published*.

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REFERENCES*