Process dynamics through the Easy Java Simulations tool (EJS)

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Introduction

The evaluation of dynamics processes in chemical engineering requires the simultaneous resolution of systems of algebraic and differential equations. These equations are considered as the dynamic model of the system, whose analytical resolution is not always possible to achieve in an easy way. The obtaining of results from the mathematical model is carried out through dynamic simulation for which the need for the development of tools that refer to the study of the process autonomously by students is raised. Virtual teaching labs are software tools that can be used locally and remotely and through the use of a model and together with an experimentation interface simulate the main aspects of a real plant, allowing the student to perform the same operations as in a laboratory traditional but virtually.

Teaching working group: virtual labs for the study of dynamic processes in chemical engineering

The general objective of the teaching working group is the development of a repository of virtual labs and interactive tools to be apply in teaching of Chemical Engineering in different courses subjects. For this, the teaching working group aims to generate resources and teaching materials that promote autonomous learning and the practical application of knowledge through advanced simulation tools programmed through Easy Java Simulations.
This work describes the creation of two remote labs using the Easy Java Simulation 6.0 tool. In both cases, they can be simulated dynamic processes in Chemical Engineering. Firstly, a photo Fenton process for the degradation of the pesticide acetamiprid (ACTM) in wastewater was implemented in continues mode with stirrer tank reactor and also the behaviour of the lab bioreactor used for enzyme-catalysed reactions. Both tools can be used online following the links placed in the figure captions of the figures 2 and 3.

Simulation of photo Fenton process in Raceway Pond Reactor

This work focuses on the development of a virtual laboratory for the study of the photo-Fenton process in raceway pond photoreactor (RPR) for the micropollutant removal of secondary WWTP effluents. The developed virtual lab is a valuable aid for both teaching and research in this subject. It helps to learn how a RPR works and to understand how the essential variables involved in the photo-Fenton process behave and interrelate between each other.

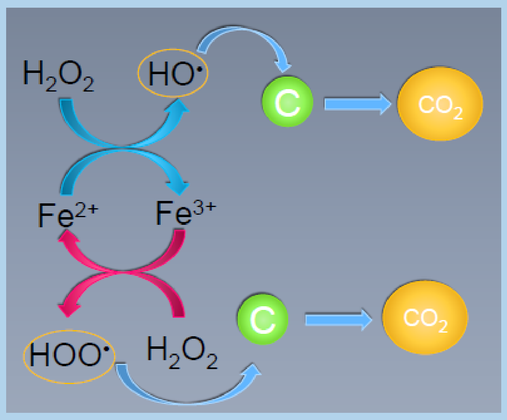

Figure 1. Photo Fenton process

As the treatment capacity of a RPR is to a great extent dependent on both hydrodynamic and geometric parameters, using this interactive tool, the performance of a specific design can be analysed. This can help either to address any issues that occur during photo-Fenton process or to provide solutions in the design of an optimal RPR.

The program start and the input data enter: RPR characteristics, ferrous ion and ACTM concentration and the liquid height. Figure 2 shows program window where the students interact it. In the same window the output data graphed (variation of the concentration of ACTM, H_2O_2, VRPA, Fe^{+2} and Fe^{+3} with time) can be followed.

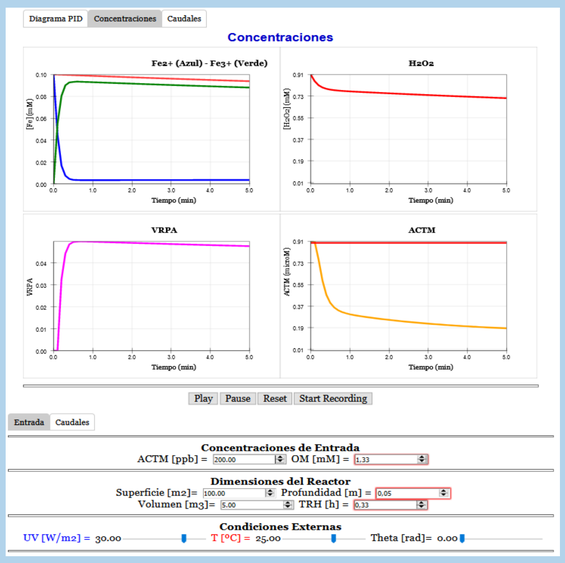

Figure 2. Photo Fenton process EJS tool.
https://w3.ual.es/docencia/idiq/PF/

Simulation of the enzymatic Continuous Stirred Tank Reactor

This research have a main goal to simulate the operation of well-mixed, continuous, and discontinuous, stirred tank bioreactor (CSTR) and a continuous plug flow bioreactor (PFBR) modelled by three units of CSTR working in series . The software allows to calculate the concentration of reagents and products at the exit from the input conditions from which the concentration of reagents ($[A]_o$, $[B]_o$), feed rate (Q), concentration and activity of the enzyme (A , E_T) for a given bioreactor volume (V_R). The virtual laboratory can be used to investigate the kinetics of a given enzyme. For this, the CSTR model would be used mainly from since the reaction rate is very easily deduced in steady state as $(-r_A) = \frac{([A]_o - [A])}{\tau}$.

The EJS code can simulate a single ideal CSTR (Figure 3.a) and three units working in series to reproduce both the conversion in non-ideal systems and the characterization of real flow in a CSTR an impulse experiment with an inert tracer. A set of three bioreactors is shown in Figure 3.b. In both cases, the EJS gives the time evolution of the concentrations of the limiting substrate and main product starting from the initial conditions represented by $[A]_o$ and $[B]_o$ inside the CSTR at t=0.

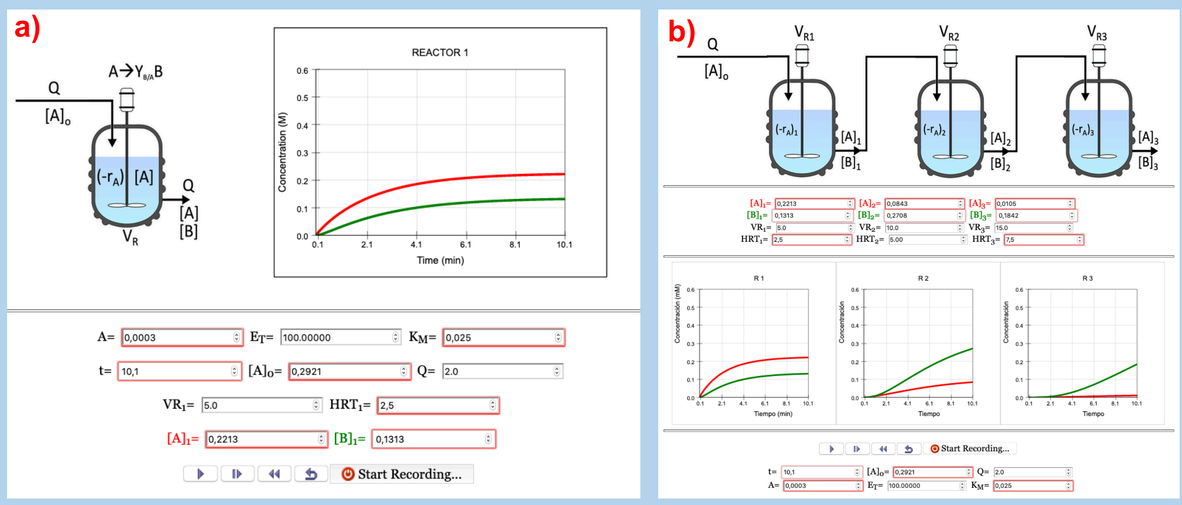

Figure 3. a) Continuous Stirred Tank Reactor
b) Bioreactors-in-series model for non-ideal flow.
https://w3.ual.es/docencia/idiq/EZM/

References

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