Virtual bioreactors programmed in Easy Java Simulations for the study of enzymatic kinetics

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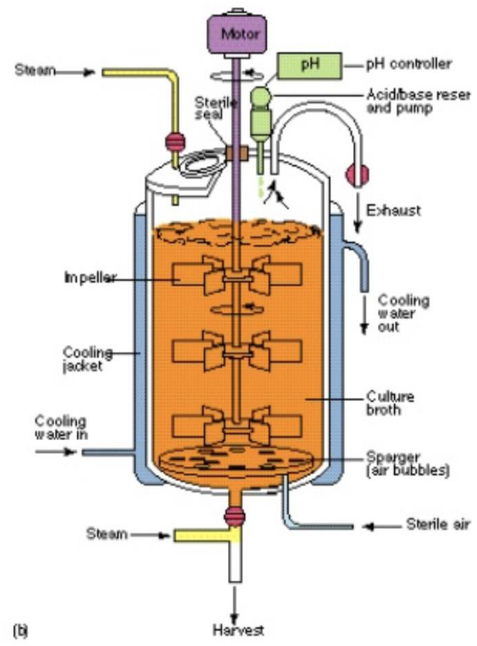
1. Introduction.

The practical classes in which the student can apply the knowledge acquired in the theory and problem classes is an indispensable complement in the scientific-technical teaching. However, in the teaching of some subjects, the implementation of lab classes, especially at a pilot or industrial scale, presents great difficulties. On the one hand, the use of equipment that can be considered industrial is expensive, requires large quantities of reagents and equipment and it is difficult to do the practices in small groups that guarantee learning for each individual student . On the other hand, in the case of enzymatic reactions, reagents and products are relatively complex and reaction monitoring is most times more difficult ald labour-demanding.



Biorreactor.

2. Teaching group “virtual laboratories for the study of dynamic processes in chemical engineering”.

The general objective of the teaching group is the development of a repository of virtual laboratories to apply in teaching of Chemical Engineering in different degrees and subjects. For this, the teaching 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.

3. Objetive.

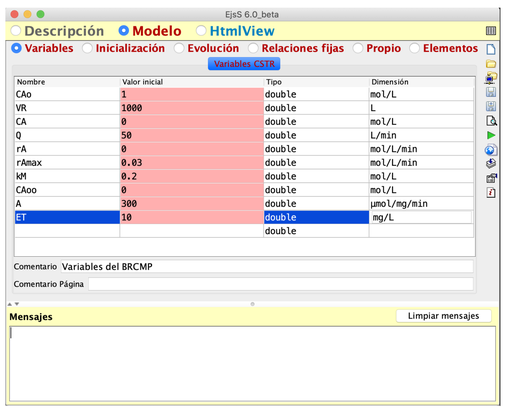
- Simulation of the operation of CSTR (well-mixed, continuous and discontinuous stirred tank bioreactor) and PFBR (continuous plug flow bioreactor). The software allows to calculate the concentration of reagents and products at the exit from the input conditions from which the concentration of reagents (C_{Ao}, C_{Bo}), 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 $(-r_A) = \frac{(C_{Ao}-C_A)}{\tau}$.
- The virtual Laboratory will allow setting up a virtual experiment (VR, C_{Ao}, Q) and will give the evolution of the limiting substrate C_A at the exit so that the student can ascertain if the steady state has been reached.
- Development of a simple real flow model, such as the series tank model, so that the student can perform impulse tracer injection experiments to determine the state of mixing of the system as well as observe the effect of a poor mixture in conversion.

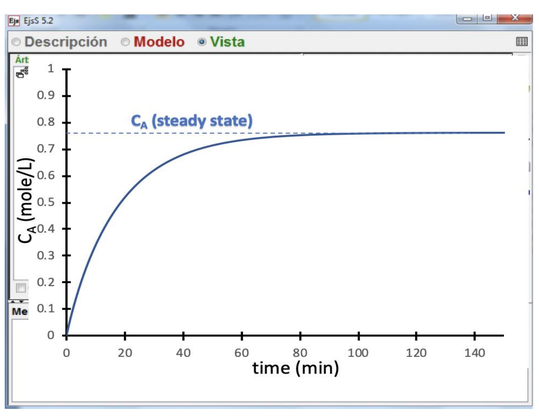
4. Equations

$$\frac{dC_A}{dt} = \frac{Q}{V_R} \cdot (C_{Ao} - C_A) - (-r_A) \qquad (-r_A) = \frac{(-r_A)_{max} \cdot C_A}{K_M + C_A}$$

$$x = \frac{C_{Ao} - C_A}{C_{Ao}} \qquad C_P = C_{Po} + Y_{P/A} \cdot C_{Ao} \cdot x$$

A: Limiting reactant, P: product, $Y_{P/A}$= yield coefficient.





3. Simulating with Easy Java/Javascript Simulations (EJS/EjsS).

- The Easy Java Simulations program was specifically designed to create simple and fast interactive scientific simulations, usually for teaching or learning purposes. It was created by the professor of the Department of Mathematics of the University of Murcia, Dr. D. Francisco Esquembre within the Open Source Physics libraries.
- Recently, EJS moved to EjsS, its JavaScript version that can run in any browser with no need of having a Java Virtual Machine installed.
- Potential EJS/EjsS users are students and teachers who have a basic knowledge of programming and can describe the models of the phenomena of each discipline in terms of algebraic and differential equations but cannot afford the large amount of time needed to create a complete graphic simulation.

4. Interactive tool for simulating bioreactor operation

- A simulation configured as a CSTR of known volume (V_R) will be used to investigate the kinetics of a virtual enzyme whose activity (A) and kinetic rate model (Michaelis, Teissier … etc) will remain hidden from the student. For the virtual experiment, the student will be instructed to set up a given enzyme concentration (E_T) and initial substrate concentration C_{Ao}. Then, the student will set up different inlet rates (Q) and let the system attain a steady state (C_A). Using the set of data thus obtained ($-r_A$ vs C_A) the student will have to propose a kinetic model and find enzyme activity (A) and the saturation constant (K_M, or equivalent parameter).

- Once known the rate model and the enzyme parameters (A, K_M), the student will be next asked to simulate the operation of an enzymatic bioreactor (CSTR or PFBR) in order to attain a given conversion (x) or propose a system to produce a required product output ($F_P=C_P \cdot Q$) given C_{Ao} and $Y_{P/A.}$
- The software will also include a model for CSTR in series so that the response of non-ideal systems can also be studied. The student will be able to assess the effect of an imperfect mixing both in CSTRs and PFBR.

5. References.

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