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Scientific Article

Dynamic Simulation of a Non-linear CSTR Using Scilab/Xcos®: a Practical Approach for Chemical Engineering Education

Simulación dinámica de un CSTR No Lineal usando Scilab/Xcos®: un enfoque práctico para la enseñanza de la Ingeniería Química

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Abstract

Understanding the dynamic behavior of chemical processes is essential for controlling industrial operation, enhancing safety, and products quality. This work provides an accessible and practical guide for students and educators to demonstrate the potential of Scilab/Xcos® as an open-source alternative to MATLAB/Simulink®, for dynamic process simulation in chemical engineering education. The study focuses on a non-linear Continuous Stirred Tank Reactor (CSTR) model, with a classic example used to illustrate the different phenomena involved in reaction engineering. Two different scenarios were simulated to analyze the transient behavior of the CSTR under different coolant temperature perturbations. In the first case, a 10 K reduction in coolant temperature led to a significant drop in reaction temperature and increase in reactant concentration. In the second case, an increase of 5 K in coolant temperature resulted in oscillatory behavior, showcasing the reactor's sensitivity to temperature changes. The presented simulation is consistent with reference values from the literature, confirming the accuracy and reliability of the Xcos® model.

***Key words*: dynamics systems, open-source, MATLAB/simulink alternatives.**

Resumen

Comprender el comportamiento dinámico de los procesos químicos es esencial para el control de procesos industriales, la mejora de la seguridad y la obtención de productos de calidad. Este trabajo proporciona una guía accesible y práctica para estudiantes y educadores, demostrando el potencial de Scilab/Xcos® como alternativa de código abierto a MATLAB/Simulink®, para la simulación dinámica de procesos en la enseñanza de la ingeniería química. El trabajo se centra en el análisis de un Reactor Continuo de Tanque Agitado (CSTR), utilizando un ejemplo clásico de la literatura para ilustrar los distintos fenómenos involucrados en la ingeniería de reacciones cuando existen no linealidades. Se simularon dos escenarios diferentes para analizar el comportamiento transitorio del CSTR bajo distintas perturbaciones en la temperatura del refrigerante. En el primer caso, una reducción de 10 K en la temperatura del refrigerante provocó una disminución significativa en la temperatura de reacción y un aumento en la concentración del reactivo. En el segundo caso, un incremento de 5 K en la temperatura del refrigerante resultó en un comportamiento oscilatorio, evidenciando la sensibilidad del reactor a los cambios de temperatura. La simulación presentada es consistente con los valores de referencia de la literatura, lo que confirma la precisión y confiabilidad del modelo en Xcos® propuesto.

Palabras clave: **sistemas dinámicos, código abierto, alternativas a MATLAB/simulink®.**

1. Introduction

The design and operation of industrial plants to produce chemicals requires a solid understanding of the dynamics systems. This field explores intricate mechanisms governing chemical reactions with time varying behaviors, facilitating the anticipation, and regulation of crucial variables like reaction rate, reaction conversion, and product selectivity. By understanding the kinetics and thermodynamics involved, engineers can design efficient processes, decrease production expenses, and mitigate environmental footprints. Moreover, process dynamics research plays a crucial role in maintaining safety standards and products quality in the chemical industry, while accelerating improvements in chemical processes (Shokry *et al*., 2020), automation technologies (Shi *et al*., 2021), and process intensification (Baldea & Edgar, 2018).

In this respect, Simulink® a toolbox from MATLAB® has helped chemical engineering students at many universities to learn dynamics and process control. Simulink® is a programming environment characterized by its block-oriented architecture, making it well-suited for dynamic system modeling and simulation. Its functionality extends to facilitating system-level design, automatic code generation, and testing and verification embedded systems. A notable attribute of Simulink® is its graphical editor and solvers, which enhance the intuitiveness and simplicity of modeling and simulation tasks compared to conventional numerical coding methods (The MathWorks, 2025).

MATLAB/Simulink® has been used widely for chemical process control analysis. It is easy to find research papers, tutorials and courses focused on the use of Simulink® for different process control applications, such as: temperature control of heat exchangers (Jin *et al*., 2021), control of chemical reactors (Muhammad *et al*., 2019) and distillation columns control (Minh, 2010). In addition, some tutorials can be found at the MathWorks website (The MathWorks, 2025) and full material of Dynamics and Control courses are available online (for example, Process Dynamics and Control by

J. Hedenren (Hedengren, 2024) or Process Dynamics, Operations and Control by B. Johnston (MIT OpenCourseWare, 2024)).

Despite the good features offered by MATLAB/Simulink®, the main disadvantage is related to licensing cost, which could limit the access to this tool in low and lower middle-income countries. Consequently, open-source alternatives represent an attractive option for dynamic system modeling and simulation. Students and educators can find dynamics and control tools that can be used in the Python programming language; however, these require a level of experience in using this language or computational tools that students do not always have. Xcos® is a dynamic systems modeler and simulator that can make up for the lack of programming experience. This powerful tool is available with Scilab®.

Scilab® offers the benefit of being an open-source simulation tool with a user-friendly interface. It encompasses numerous mathematical functions and allows the integration of programs from other languages, such as C++ and Fortran. Additionally, it features a control-oriented toolbox known as Xcos®, which employs a block-oriented programming approach. Xcos® enables the creation of mathematical models graphically, utilizing fundamental computing blocks in discrete and continuous time domains (Dassault Systèmes, 2024).

The Autonomous University of Chihuahua (Universidad Autónoma de Chihuahua, UACH) in Mexico, offers a process dynamics and control course at the ninth semester (the last semester) in the undergraduate Chemical Engineering and Food Engineering programs. This subject is a chemical engineering course commonly offered in other universities worldwide at the end of the program, as mentioned by Moodley (Moodley, 2020).

Although, the exploration of chemical reactor dynamics starts with the chemical reactor design course during the third year of the chemical engineering program at the UACH, the process dynamics and control course is focused on understanding the dynamic performance and control strategies of different process units such as: mixing tanks, separation columns, heat exchangers, boilers, and chemical reactors. An important part of the course is that the students gain knowledge about transient behavior of the processes to evaluate different scenarios that can be found in industry related to normal and abnormal operation conditions. To achieve this, the use of computational tools for modeling and simulating chemical processes in dynamic states is both crucial and necessary in the classroom. The same assertion has been made by other authors such as, Moodley (2020), Vieira *et.al.* (2019), and Henrique *et.al.* (2018).

According to Vieira *et.al.* (2019), Xcos® is an excellent option for studying dynamic simulations. However, there is a lack of research papers focused on training and demonstrating the utility of Xcos® for academic purposes, with most information concentrating on process control.

Hence, the aim of this paper is to present a useful guide for students and professors interested in the field of chemical process dynamics by using the Scilab/Xcos® programming environment. Also, the paper brings a comprehensive derivation of the dynamic mass and energy balance equations involved in the system, by solving a classical non-linear Continuous Stirred Tank Reactor (CSTR) dynamics example, described in the workhorse book of Process Dynamics and Control written by Seaborg, *et.al.* (2016).

To facilitate reading, the paper is divided into the following sections: in Section 2 an example of dynamic assessment process is presented, and mathematical model and implementation in Xcos® is also presented. In section 3, the simulations results can be found. Finally, the conclusions are given in section 4.

2. Materials and Methods

The study of continuous stirred-tank reactors in chemical engineering programs is of a great importance because they are widely used in different industrial applications, such as: pharmaceuticals (Hu, 2021), polymers manufacturing (Wang *et al*., 2018), in biotechnology to treat petroleum wastewater (Pugazhendi *et al.,* 2017), and some novel applications such as clean hydrogen production (Ghimire *et al*., 2015).

Another important characteristic is that CSTR models are simpler than other reactors such as tubular and packed-bed reactors. Hence, the study of continuous stirred-tank reactors offers a practical means to demonstrate modeling principles for chemical reactors in an educational setting.

2.1. Model description

For this study, a non-isothermal continuous stirred-tank reactor was modeled and simulated, adapted from (Seborg *et al*., 2016). In this setup, a liquid-phase chemical reaction is studied, where species A irreversibly transforms into species B. The reaction equation can be represented as follows:

$$A \rightarrow B \qquad \text{Eq. (1)}$$

An assumption is that the reaction rate is determined by the concentration of component A, following first-order reaction kinetics (Eq. 2).

$$r = kC_A \qquad \text{Eq. (2)}$$

Where (r) is the reaction rate, (k) is the reaction rate constant, and (C_A) is the molar concentration of the reactant A.

For single-phase reactions, it can be assumed that the rate constant depends only on the reaction temperature that it can be described by the Arrhenius equation, expressed by Eq. (3).

$$k(T) = A \exp\left(-\frac{Ea}{RT}\right) \qquad \text{Eq. (3)}$$

Where (A) is the frequency factor, (E_a) is the activation energy, (R) is the ideal gas constant, and (T) is the absolute reaction temperature.

Regarding Eqs. (2) and (3), these are classified as semi-empirical relations since the parameters (A) and (Ea) are obtained by fitting experimental data.

In Fig. 1, the schematic diagram of the CSTR studied in this work is shown. As can be seen, only component A is fed to the reactor at a certain flow rate (q), at temperature (T_f) with a molar

concentration (C_{A_f}). The outlet stream exits the reactor at a flow rate of (q), at the reaction temperature (T) with a concentration of (C_A). To keep reaction at the desired temperature (nominal value), a cooling fluid is fed through the cooling coil at temperature (T_c).

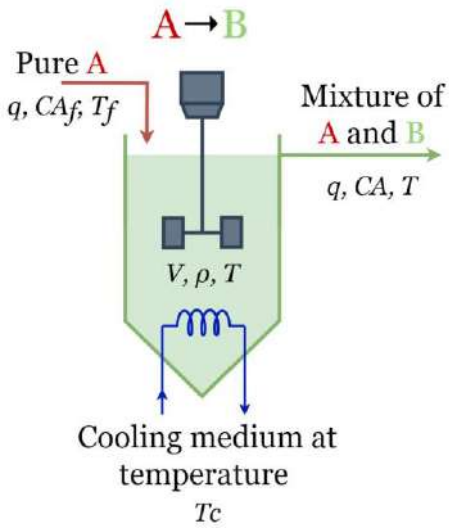


Figure 1. Continuous Stirred Tank Reactor adapted from Seaborg *et.al.* (2016).
Figura 1. Reactor Continuo de Tanque Agitado adaptado de Seaborg *et al*. (2016).

2.2 Mathematical model

This section provides the dynamic derivation of the mass and energy balance equations based on fundamental principles.

Mass balance

The derivation of the ordinary differential equation that describes the accumulation rate of the chemical reactants is based on several ideal assumptions (Seborg *et al.*, 2016):

- A complete mixing is considered.
- Feed and products have constant densities, denoted as (ρ).
- Reaction takes place at constant volume (V).

Under the previous assumptions, the general mass balance equation can be expressed in the form shown by Eq. (4).

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{G}_i \qquad \text{Eq. (4)}$$

The derivative term $\left(\frac{dM}{dt}\right)$ in Eq. (4) represents the material accumulation in the system, ($\dot{m}_{in}$) and ($\dot{m}_{out}$) are the inlet and outlet mass flow rates, respectively, ($\dot{G}_i$) is the generation rate of any chemical

species due to chemical reactions. Since (V) and (ρ) are constants, then the mass (M) and mass flow rate ($\dot{m}$) can be expressed in the form of Eqs. (5) and (6), respectively.

$$M = \rho \cdot V \quad \text{Eq. (5)}$$

$$\dot{m} = \rho \cdot q \quad \text{Eq. (6)}$$

On the other hand, the rate of generation and consumption of the reactant (A, in this reaction) is based on reaction kinetics; see Eq. (2). Assuming a well-mixed reactor condition, the reaction rate (r_i) does not change with respect to the reactor position. Then, the generation rate of any species can be expressed in the form of Eq. (7).

$$\dot{G}_i = r_i V \quad \text{Eq. (7)}$$

For this example, a first-order reaction is considered with respect to A; hence, the kinetic equation is given by Eq. (8)

$$r_A = kC_A \quad \text{Eq. (8)}$$

Substituting Eqs. (5–8) into Eq. (4) leads to Eq. (9):

$$\frac{d(\rho V)}{dt} = \rho q_i - \rho q - VkC_A \quad \text{Eq. (9)}$$

Where (q_i) and (q) are the inlet and outlet volumetric flows, respectively.

Finally, since (V) and (ρ) are constants, the inlet and outlet volumetric flow rates (q_i and q) are equal, and this assumption must be satisfied at all the time (Seborg *et al*., 2016).

With the previous assumptions, the unsteady-state component balance for specie A (in molar units) is described by Eq. (10).

$$V\frac{dC_A}{dt} = q\left(C_{A_i} - C_A\right) - VkC_A \quad \text{Eq. (10)}$$

Energy balance

To derive the energy balance equation, the following assumptions are needed (Seborg *et al*., 2016):

- The thermal capacitance of the coolant and the wall of the heat transfer tubes is negligible compared to the thermal capacitance of reaction species inside the reaction tank.
- Uniform coolant temperature distribution is considered, and it is denoted as (T_c). Therefore, any temperature changes in coolant temperature when passes through the tubes is neglected.
- The heat of mixing is negligible compared to the reaction enthalpy.
- Thermal losses to the ambient and shaft work are neglected.

According to the assumptions, the dynamic general energy balance equation is presented in Eq. (11).

$$\frac{dE}{dt} = \dot{E}_{in} - \dot{E}_{out} + \dot{E}_g - \dot{E}_c \quad \text{Eq. (11)}$$

Where derivative term $\left(\frac{dE}{dT}\right)$ represents the energy accumulation in the system, $(\dot{E}_{in})$ and $(\dot{E}_{out})$ are the energy flow that enters and exits the system, and $(\dot{E}_g)$ and $(\dot{E}_c)$ is the rate of reaction heat.

To account the energy accumulation in the system, and the energy flow through the system, Eqs. (12-14) are used in terms of density, volume and enthalpy.

$$E = M \cdot h = \rho \cdot V \cdot h \quad \text{Eq. (12)}$$

$$\dot{E}_{in} = \dot{m}_{in} \cdot h_{in} = \rho \cdot q_i \cdot h_{in} \quad \text{Eq. (13)}$$

$$\dot{E}_{out} = \dot{m}_{out} \cdot h_{out} = \rho \cdot q \cdot h_{out} \quad \text{Eq. (14)}$$

Where (M) is the reaction mass, $(\dot{m}_{in})$ and $(\dot{m}_{out})$ are the inlet and outlet mass flow rates, and (h), (h_{in}) and (h_{out}) are the inlet and outlet specific enthalpies.

The rate of heat generation $(\dot{Q}_{gen})$ due to the chemical reaction is accounted by Eq. (15), and the heat transfer between the reaction and the coolant is expressed by Eq. (16).

$$\dot{Q}_{gen} = (-\Delta H_r) V k C_A \quad \text{Eq. (15)}$$

$$Q = UA(T_c - T) \quad \text{Eq. (16)}$$

Where $(-\Delta H_r)$ is the change of enthalpy of reactants and products, (VkC_A) is the reaction rate at constant volume, (U) represents the overall heat transfer coefficient, (A) denotes the heat transfer area, (T_c) and (T) are the average coolant and reaction temperatures, respectively.

Substituting Eqs. (12-16) in Eq. (11), the energy balance equation takes the form of Eq. (17), where specific enthalpies can be written as the product of $(Cp \cdot T)$.

$$\rho V Cp \frac{dT}{dt} = \rho q Cp\left(T_f - T\right) + (-\Delta H_r) V k C_A + UA(T_c - T) \quad \text{Eq. (17)}$$

2.3 Model implementation in Xcos®

The intuitive graphical editor in Xcos® simplifies the representation of mathematical models through block diagrams, where each block corresponds to a predefined function or a user-defined custom function. These blocks connect seamlessly within the interface, enabling straightforward system design and analysis (Dassault Systèmes, 2024). In this section a brief description of the blocks used on the CSTR model is presented.

Xcos® Blocks description

To guide readers in creating the block diagram shown in Fig. 2, Table 1 provides a description of each object used in this work. The block descriptions are available in the *palette browser* within Xcos®.

CSTR model

The CSTR model, which includes Eqs. (3, 10, and 17), corresponds to a coupled set of differential and algebraic equations. Each equation was implemented in separate subsystems (*SUPER_f blocks*) to improve the understanding of the coupled system and facilitate the manipulation of the variables involved, as shown in Fig. 2.

The illustration of Fig. 2 shows the interaction between subsystems. The initial guess is based on the steady-state conditions for reaction temperature (T_0) and specie A concentration (C_{A_0}). Under these conditions, the reaction rate constant (k) is computed within the *Arrhenius Equation Subsystem* and then passed to the *Mass and Energy Balance Subsystems* to update the reaction temperature and concentration. This process repeats multiple times until the simulation is complete. The system integrates user-defined functions with built-in Xcos blocks for mass and energy balances. The mass balance equation is solved through a dedicated subsystem (highlighted in magenta), while the energy balance is handled in a separate module (in red). The data flow arrows represent the directional exchange of variables (e.g., concentration, temperature) between the subsystems and the main function block.

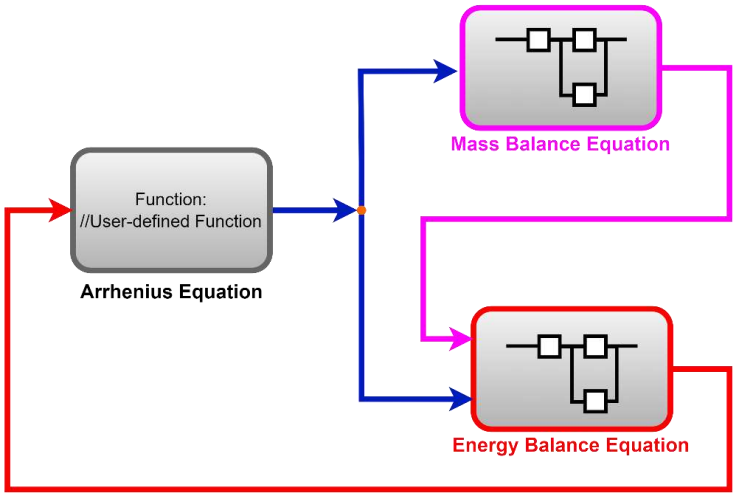
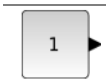
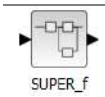
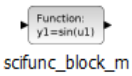


Figure 2. Diagram of the coupled system implemented in Xcos® for the dynamic simulation of a Continuous Stirred Tank Reactor (CSTR).

Figura 2. Diagrama del sistema acoplado implementado en Xcos® para la simulación dinámica de un reactor continuo de tanque agitado (CSTR).

Table 1. Description of the blocks used from *palette browser* in Xcos®.
Tabla 1. Descripción de los bloques utilizados del *palette browser* en Xcos®.

Block name	Description
	This block is an integrator. The output y is the integral of the input u at the current time step t.
	Set constant value block. This block allows setting a numeric constant value.
	This block performs addition or subtraction on scalar, vector or matrix inputs. The input datatype is set with the datatype parameter. The *number of inputs or sign vector* parameter defines the number of inputs and operation. For a single vector's input, the block collapses the elements of the vector. Vectors/matrices inputs must have the same size.
	This block computes element-wise multiplication or division of its vector inputs. The number of inputs and operation are specified with the number of inputs or sign vector parameter. To *multiply/divide* the input u_i, set in this parameter a vector k with $+1$ *(multiply)* or -1 *(divide)* for the input u_i.
	The unique output of this block generates a regular train of events that are scheduled by parameter *period* in seconds. The starting date of events generation can be set in seconds with the *Initialization Time* parameter.
	The Scope block displays its input with respect to simulation time. Both axes have a common range. The Scope allows you to adjust the amount of time and the range of input values displayed. It has the feature to scale the graph at runtime.
	This block opens a new Xcos® window for editing a new block diagram. This diagram describes the internal functions of the super block. Super block inputs and outputs (regular or event) are designated by special (input or output) blocks.
	This block can realize any type of Scicos block. The function of the block is defined interactively using dialogue boxes and in Scilab® language. During simulation, these instructions are

interpreted by Scilab®; the simulation of diagrams that include these types of blocks is slower

Simulation parameters

The effect of sudden changes in coolant temperature (T_c), was analyzed by replicating both positive and negative step changes in (T_c), as reported in Seborg *et al*. (2016).

Table 2 presents key parameters and nominal operating conditions for the Continuous Stirred Tank Reactor. The system is described by ordinary differential equations (ODEs), with two state variables: reactant concentration (C_A) and reactor temperature (T). The cooling water temperature (T_c) serves as the manipulated variable.

Table 2. Simulation parameters (Seborg *et al*., 2016).
Tabla 2. Parámetros de simulación (Seborg *et al*., 2016).

Parameter	Symbol	Value	Units
Activation energy	E_a	72,750	J/mol
Arrhenius pre-exponential	k_0	$7.2x10^{10}$	min^{-1}
Gas constant	R	8.314	$J/mol \cdot K$
Reactor volume	V	100	L
Density	ρ	1000	g/L
Heat capacity	Cp	0.239	$J/g \cdot K$
Enthalpy of reaction	ΔH_r	-50,000	J/mol
Heat transfer coefficient	UA	50,000	$J/min \cdot K$
Feed flowrate	q	100	L/min
Feed concentration	C_{A_f}	1.0	mol/L
Feed temperature	T_f	350	K
Initial concentration	C_{A_0}	0.5	mol/L
Initial temperature	T_0	350	K
Coolant temperature	T_C	300	K

Mass balance equation subsystem configuration

To implement the mass balance equation in Xcos® environment, Eq. (10) needs to be rearranged as follows: the volume divides the equation to have only the derivative term at the left-hand side of the equation. As a result, both terms on the right-hand side of Eq. (10) are also divided by the volume (V), yielding a new equation, given in Eq. (18).

$$\frac{dC_A}{dt} = \frac{q}{V}\left(C_{A_i} - C_A\right) - kC_A \qquad \text{Eq. (18)}$$

The block diagram for Eq. (18) that is within the subsystem called *Mass Balance Equation*, is presented in Fig. 3. The nominal parameters (q), (V), and (C_{A_f}) are modeled using constant blocks since their values remain unchanged during the simulation. To declare their respective value, the *set context* box that can be found on the simulation tab was used. About algebraic operations, they are represented by their respective addition, subtraction, multiplication and division blocks. To help readers understand how these operations were performed, labels were added to the corresponding blocks to indicate the type of computation carried out, see Fig. 3.

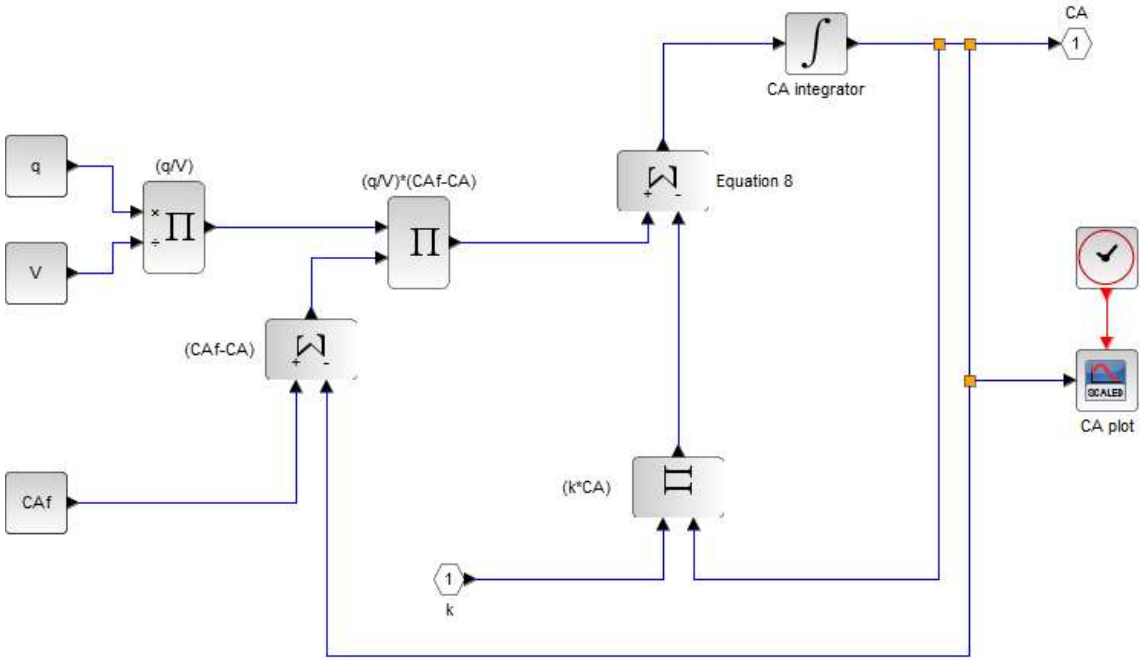


Figure 3. Block diagram in Xcos® representing the dynamic implementation of the mass balance equation for the Continuous Stirred Tank Reactor (CSTR).

Figura3. Diagrama de bloques en Xcos® que representa la implementación dinámica de la ecuación de balance de masa para el Reactor de Tanque Agitado Continuo (CSTR).

In Fig. 3 is shown the problem model. The model incorporates key input parameters such as flow rate (q), reactor volume (V), and feed concentration (C_A). The expression $(q/V)(CA_f - C_A)$ represents the convective mass transport, and the term (kC_A) accounts for the first-order reaction kinetics. The output concentration (C_A) is obtained through numerical integration and plotted in real time using the Scope block.

The *set context* box allows variable definition and mathematical operations to simplify variable manipulation, see Fig. 4.

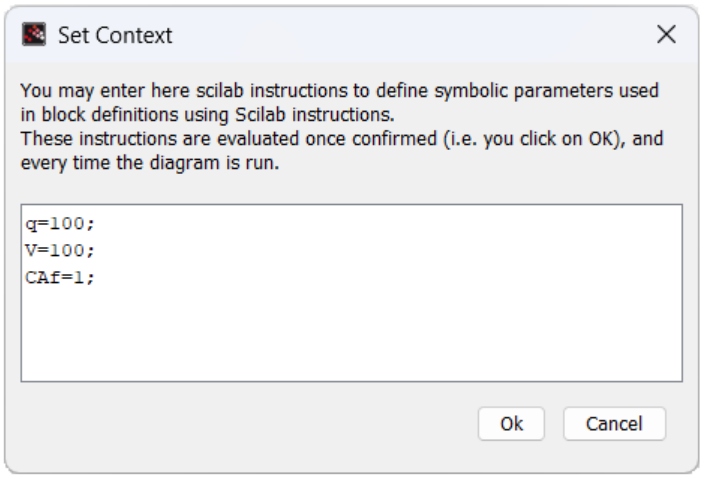


Figure 4. Variable definition in *set context* for the mass balance equation.
Figura 4. Definición de variables en *set context* para la ecuación de balance de masa.

Finally, the integrator is set up with the initial condition $C_{A_0} = 0.5\ mol/L$. This action can be done by clicking on the integrator block and typing the desired value on the *initial condition* blank space, see Fig. 5.

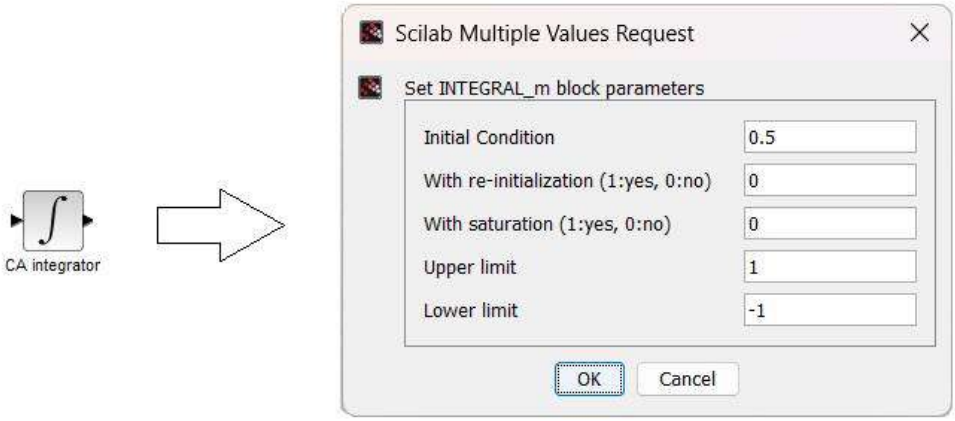


Figure 5. Initial condition set up for the C_A integrator block.
Figura 5. Configuración de la condición inicial para el bloque integrador C_A.

Energy balance equation subsystem

Analogous to the mass balance equation, Eq. (17) must be solved to isolate the derivative term. To achieve this, Eq. (17) is divided by the product of (ρVCp), resulting in a new equation, Eq. (19).

$$\frac{dT}{dt} = \frac{q}{V}(T_i - T) + (-\Delta H_r)\frac{kC_A}{\rho Cp} + \frac{UA}{\rho VCp}\ (T_c - T) \qquad \text{Eq. (19)}$$

In Fig. 6, the block diagram to solve Eq. (19) is presented. In this case the nominal parameters were also introduced as constant blocks, such as: $q, V, T_f, \Delta H_r, \rho, UA$, and Cp.

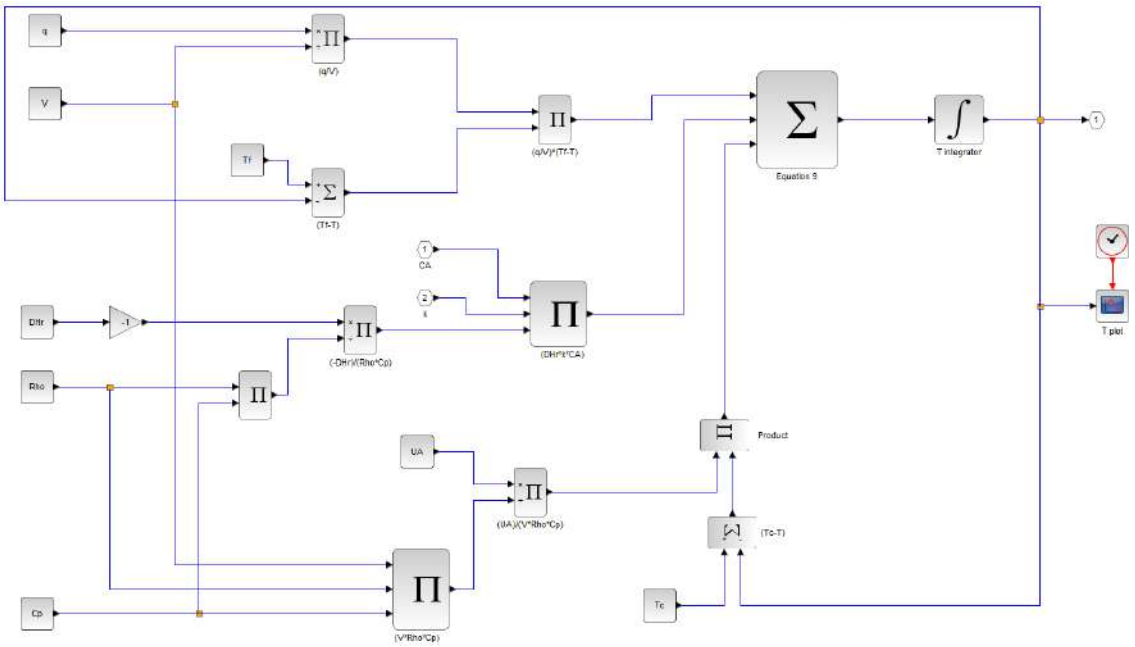


Figure 6. Xcos® block diagram implementing the energy balance equation for the Continuous Stirred Tank Reactor (CSTR).

Figura 6. Diagrama de bloques de Xcos® que implementa la ecuación de balance de energía para un Reactor de Tanque Agitado Continuo (CSTR).

In Fig. 6 is shown how the model dynamically calculates the reactor temperature (***T***) by integrating contributions from convective heat exchange $(q/V)(T_f - T)$, heat generated by the reaction $(-\Delta H_r kC_A)$ and heat transfer with the cooling medium $(UA/V\rho Cp)$. The values of the nominal constant parameters were also set using the *set context* box (see Fig. 7).

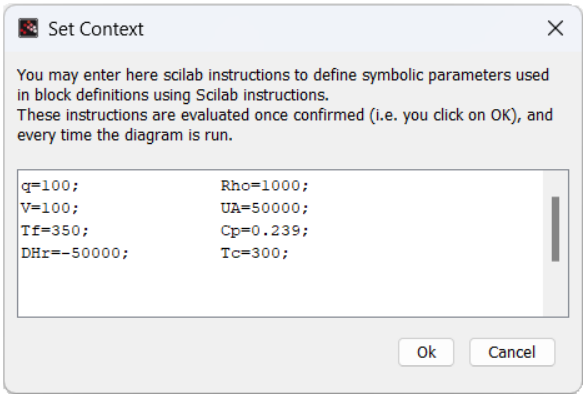


Figure 7. Variable definition in *set context* box for energy balance equation.
Figura 7. Definición de variables en *set context* para la ecuación de balance de energía.

For the reaction temperature integrator, the initial condition was set to 350 K, as shown in Fig. 8.

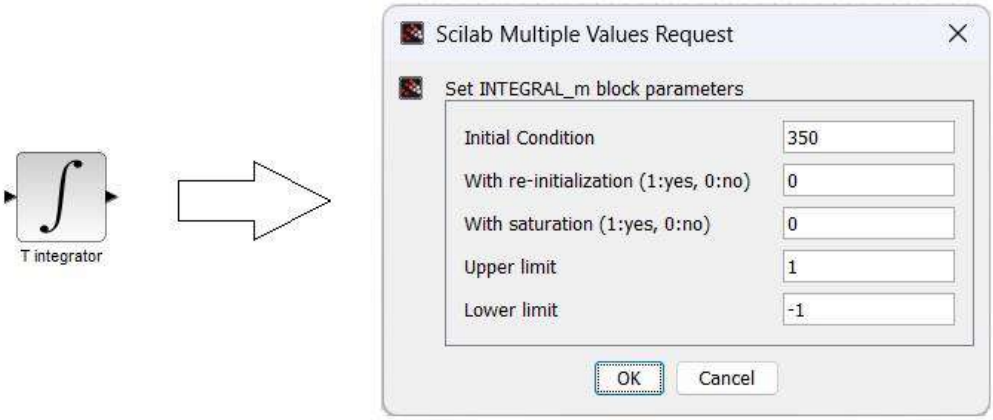


Figure 8. Initial condition set up for reaction temperature integrator block.
Figura 8. Configuración de la condición inicial para el bloque integrador de temperatura de reacción.

Arrhenius equation block

The Arrhenius equation is an exponential function that depends on temperature (Eq. 3). Each time the reaction temperature changes, the reaction rate constant must be recalculated. In Xcos®, solving this equation requires utilizing the user-defined function *sfunc_block_m*.

Double-clicking the *sfunc_block_m* opens a new configuration window. The first two entries, *input port sizes* and *output port sizes*, should be set to [1,1] and [1,1], respectively. This configuration indicates that a single input variable, the reaction temperature (T) from the Energy Balance Subsystem enters the block, while a single output variable, the specific rate constant, exits. Once the input and output port sizes are defined, click *OK* to proceed.

The previous action displays a new box where the function is introduced as follows: on the top of the box the name of the function is written as *Arrhenius Equation*, then the inlet variable (T) that comes from the *Energy Balance* equation is defined as *Global T*. If more input variables are needed, all of them must be settled as global variables.

To solve a time-dependent function in Xcos®, it must be expressed in the form $y = u$. The Arrhenius equation is then solved in the form of Eq. (20).

$$y_1 = (u_2) \cdot \exp\left(\frac{u_3}{u_4 \cdot u_1}\right) \quad \text{Eq. (20)}$$

Where $y_1 = k(T)$;

$u_2 = A$;

$u_3 = E_a$;

$u_4 = R$;

$u_1 = T$

Once the function is defined, click *ok* to continue. The new box, the global variable (T) is rewritten for initialization and click *ok*. If more input variables are needed, they must be declared here for their respective initialization.

The fourth box is used to create additional commands such as: create graphics, export data open/close graphics, etc. In this case the box has been left in blank, due to additional instructions are not necessary. Finally, the last box can be used to define restriction for input, output and state variables if needed, but in this case, it was also left in blank. The whole process of the user-defined function configuration is depicted in Fig. 9.

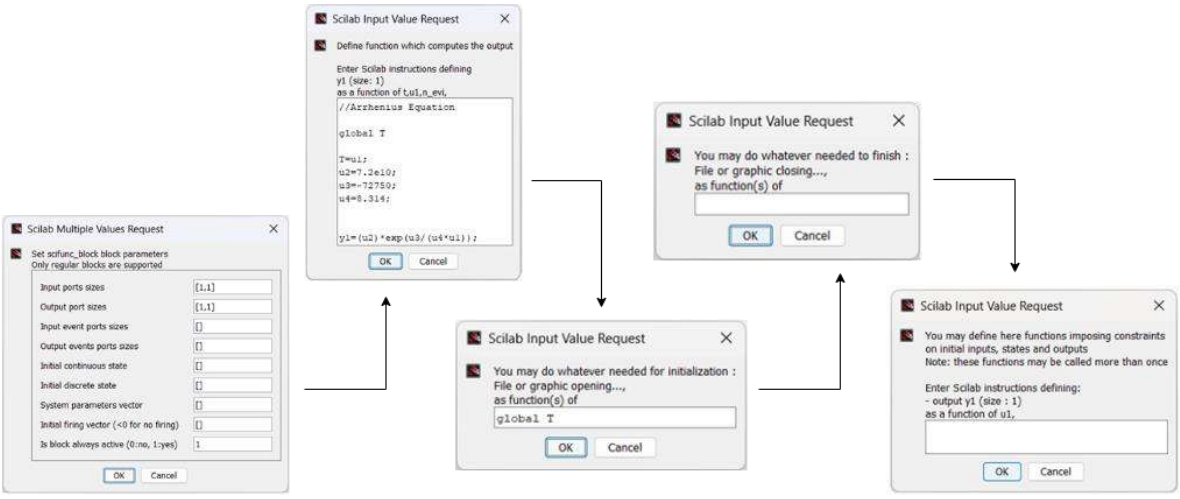


Figure 9. The Arrhenius equation configuration using the *sfunc_block_m*.
Figura 9. Configuración de la ecuación de Arrhenius utilizando el *sfunc_block_m*.

3. Results and discussion

To analyze the transient behavior of the CSTR model presented in the previous section, two different scenarios were simulated as follows: for the first case, enhanced cooling was simulated by modifying T_c from 300 K to 290 K. The second case focuses on reducing the cooling rate, accomplished by increasing T_C from 300 K to 305 K. For both cases, the simulation time was set to 10 minutes.

In the first case, decreasing the coolant temperature to 290 K has two major effects. First, the reaction temperature drops by approximately 37 K, reaching a new steady-state value of 312.6 K. Second, the molar concentration of the reactant (C_A) increases from 0. mol/L to a new steady-state value of 0.952 mol/L.

For the second simulation, when the cooling jacket temperature is set at 305 K, the CSTR exhibits sustained oscillations due to the exothermic nature of the reaction and its strong temperature dependence. As the temperature spikes, the reaction accelerates quickly consuming reactant A. Once the concentration drops, heat generation decreases, allowing the reactor to cool. The continuous feed then restores the amount of A, initiating a new cycle.

This nonlinear feedback between reaction kinetics and heat removal leads to self-sustained oscillations in temperature and concentration. As explained by Seborg *et al.* (2016), such behavior is not unusual in chemical reactors, particularly under marginal or critical operating conditions. Small variations in parameters like the coolant temperature, inlet concentration, or activation energy can drastically shift the system from steady-state to oscillatory or even unstable regimes.

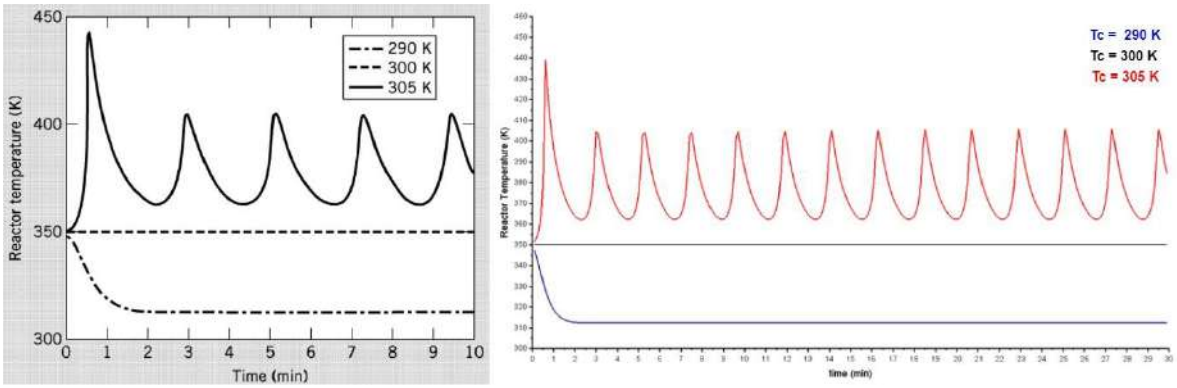


Figure 10. Reactor temperature response due to coolant temperature changes (Tc), nominal temperature of 300 K. Left side represents the reference results from Seborg *et al.* (2016) and the right side shows the results obtained with Xcos®.

Figura 10. Respuesta de la temperatura del reactor debido a cambios en la temperatura del refrigerante (Tc), con una temperatura nominal de 300 K. El lado izquierdo representa los resultados de referencia de Seborg *et al*. (2016), y el lado derecho muestra los resultados obtenidos con Xcos®.

According to this, the results obtained with Xcos® align with the reference values, confirming that the CSTR model simulated in this study accurately represents the reference model reported by

Seborg *et al*. (2016). Figs. 10 and 11 present a graphical comparison between the reference results and the previously discussed simulations.

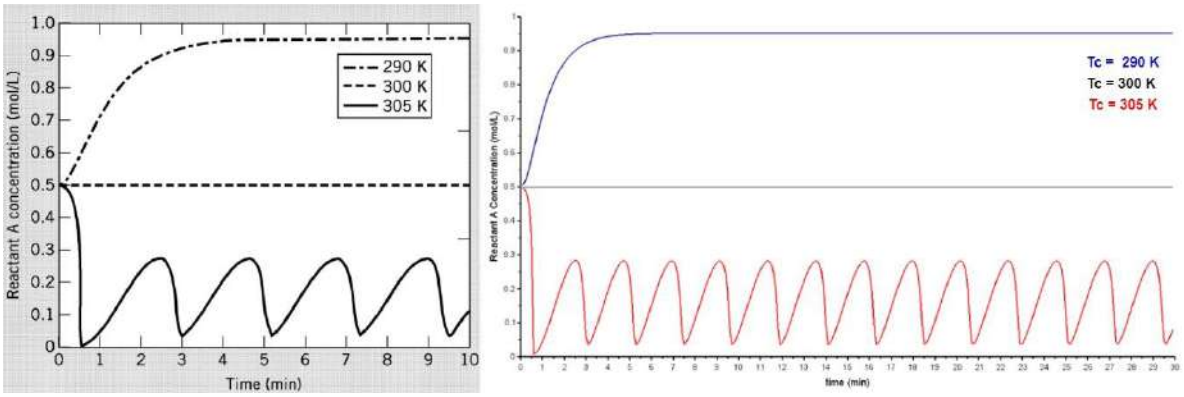


Figure 11. Concentration response due to coolant temperature changes (Tc), nominal temperature 300 K. Left side represents the reference results from Seborg *et al*. (2016) and the right side shows the results obtained with Xcos®.

Figura 11. Respuesta de la concentración debido a cambios en la temperatura del refrigerante (Tc), temperatura nominal de 300 K. El lado izquierdo representa los resultados de referencia Seborg *et al*. (2016), y el lado derecho muestra los resultados obtenidos con Xcos®.

4. Conclusions

This study explored the use of Xcos® for solving dynamic chemical engineering problems. Specifically, the dynamics of a continuous stirred tank reactor (CSTR) were analyzed, including model description, mathematical formulation, and Xcos® implementation.

Although, the use of Scilab/Xcos® is not new in research or academia, most of the research papers are focused on dynamics for control purposes of specific problems in which it is assumed that readers have certain knowledge on the topic to understand both mathematical models and implementation. Hence, the structure of this paper was intended to be a practical guide describing the steps to follow for dynamic modeling and simulation with Xcos®, especially for students and educators interested in dynamic systems.

The simulator was validated using a well-known example from Seborg *et al.* (2016), a widely used textbook in process dynamics and control courses. The simulation results closely matched the reference values, confirming the accuracy of the model. Therefore, this model can serve as a reliable reference for educational projects and research activities related to chemical reaction engineering.

Currently, our research group is developing different unit operation simulators that are commonly studied in chemical engineering programs. The research group aims to offer a wide range of models for analyzing full plant process dynamics and supports the teaching process using open-source tools.

Hence, we encourage readers to contact the corresponding author for access to the simulator or for further guidance on how to implement the models discussed in the paper. The authors are open to providing support for specific simulations, answering technical questions, and offering insights on adapting the simulator to different case studies or research needs. Reaching out can help ensure the correct use of the simulator and facilitate collaboration on improvements or extensions.

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Declaration of Competing Interest

The authors declare that there are no known financial conflicts of interest or personal relationships that could have influenced the research presented in this paper.

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