

# Continuous Stirred Tank Reactor (CSTR) Dynamics Simulation

## Abstract

Continuous Stirred Tank Reactors (CSTRs) play a pivotal role in the chemical and process industries due to their steady-state operational capabilities. This study delved into the influence of initial temperature on the dynamics of a CSTR system. Focusing on the reaction  $A+B\rightarrow P$ , which follows a second-order rate law, the role of temperature in reaction kinetics, as described by the Arrhenius equation, was examined. The study explored the initial temperature impact on the reactant and product concentrations and the overall temperature by simulating the reactor's behavior using MATLAB and varying the initial temperature. Key findings revealed that the initial temperature profoundly affects reaction rates, time to reach steady states, and the overall behavior of the reactor. Multiple steady states were observed in some cases, highlighting the complexities inherent in reactor dynamics. This research underscores the importance of understanding the implications of initial temperature, providing crucial insights for optimizing reactor performance, safety, and design strategies in industrial applications.

## 1. Introduction

Continuous Stirred Tank Reactors (CSTRs) are among the most common reactors in the chemical and process industries. Their versatility and capacity for steady-state operations make them particularly suitable for various reactions. In a CSTR, the reactants are continuously fed into the reactor while the products are continuously removed, ensuring a uniform composition and temperature throughout the reactor volume. CSTR reactor contrasts with other reactor types, such as batch reactors, where all reactants are loaded initially and left to react, and the products are removed at the end.

Various factors, including the type of reaction, rate constants, feed compositions, and initial conditions, can influence the dynamics of a CSTR. The present study focuses on the reaction  $A+B\rightarrow P$ , which follows a second-order rate law. Given the critical role temperature plays in reaction kinetics, mainly as dictated by the Arrhenius equation, understanding the impact of initial reactor temperature on system dynamics is paramount.

This simulation study aims to delve deep into the reactor's behavior by varying the initial temperature. By doing so, we seek to understand how this factor influences concentrations of reactants and products over time and the reactor's overall temperature profile. Further, given the complex interplay of reaction kinetics, heat effects, and mass transfer, the intriguing possibility exists to observe multiple steady states under certain conditions.

Through this exploration, we aim to understand the fundamental behavior of our CSTR system under varying initial conditions and glean insights that can guide operational and design strategies for real-world applications.

## 2. Theoretical Background

Continuous Stirred Tank Reactors (CSTRs) are a cornerstone in the realm of chemical engineering due to their ubiquity in many chemical processes. To understand the intricacies of their behavior, one must delve into the fundamental governing equations and principles underlying their operation. This section elucidates the theoretical framework pertinent to our CSTR study.

## 2.1 Reaction Kinetics

The reaction under consideration,  $A+B \rightarrow P$ , is governed by a second-order rate law, mathematically represented as:

$$r = k \times C_A \times C_B$$

Where  $r$  is the rate of reaction,  $k$  is the rate constant, and  $C_A$  and  $C_B$  are the concentrations of reactants A and B, respectively. The Arrhenius equation defines the relationship between the rate constant  $k$  and temperature  $T$ :

$$k = A_i \times \exp(-E_i / RT)$$

Here,  $A_i$  is the frequency factor or pre-exponential factor,  $E_i$  is the activation energy, and  $R$  is the universal gas constant. This equation underscores the sensitivity of reaction rates to temperature, an aspect that becomes pivotal in our study.

## 2.2 Material Balances

Overall mass balance for a CSTR can be written as:

$$\text{Accumulation} = \text{Inlet} - \text{Outlet}$$

$$\frac{d\rho V}{dt} = \rho F_{in} - \rho F$$

$$\frac{dV}{dt} = F_{in} - F$$

Where  $\rho$  denotes mixture density,  $F$  represents the volumetric flow rate, and  $V$  represents the reactor volume.

For any reactor, the dynamics of the components are determined by material balances.

$$\text{Accumulation} = \text{Inlet} - \text{Outlet} + \text{Generation} - \text{Consumption}$$

$$\frac{dn_A}{dt} = \dot{n}_{A_{in}} - \dot{n}_{A_{out}} - r_A V$$

$$\frac{dVC_A}{dt} = F_{in} C_{A_{in}} - F_{out} C_{A_{out}} - r_A V$$

$$C_A \frac{dV}{dt} + V \frac{dC_A}{dt} = F_{in} C_{A_{in}} - F_{out} C_{A_{out}} - r_A V$$

$$C_A (F_{in} - F_{out}) + V \frac{dC_A}{dt} = F_{in} C_{A_{in}} - F_{out} C_{A_{out}} - r_A V$$

$$V \frac{dC_A}{dt} = F_{in} (C_{A_{in}} - C_A) - r_A V$$

For our CSTR system, the balances for reactants A and B and product P are represented as:

$$\frac{dC_A}{dt} = \frac{F_{in}}{V} (C_{A_{in}} - C_A) - C_A C_B A_i \exp(-E_i / RT)$$

$$\frac{dC_B}{dt} = \frac{F_{in}}{V} (C_{B_{in}} - C_B) - C_A C_B A_i \exp(-E_i / RT)$$

$$\frac{dC_P}{dt} = \frac{F_{in}}{V} (C_{P_{in}} - C_P) + C_A C_B A_i \exp(-E_i / RT)$$

Where  $C_A$ ,  $C_B$  and  $C_P$  are A, B and P feed concentrations, respectively.

### 2.3 Energy Balance

Being an adiabatic system, the CSTR does not exchange heat with its surroundings. The energy dynamics are thus steered by the heat brought in by the feed, the heat taken out by the product, and the heat generated or absorbed by the reaction. Energy balance can be mathematically represented by:

$$Accumulation = Inlet - Outlet + Generation - Consumption$$

$$\frac{d(V\rho c_p T)}{dt} = F_{in}\rho c_p T_i - F\rho c_p T + (-\Delta H)(-r_A)V$$

$$\frac{d(VT)}{dt} = F_{in}T_i - FT + \frac{(-\Delta H)(-r_A)V}{\rho c_p}$$

$$T \frac{dV}{dt} + V \frac{dT}{dt} = F_{in}T_i - FT + \frac{(-\Delta H)(-r_A)V}{\rho c_p}$$

$$\frac{dT}{dt} = \left( \frac{F_{in}}{V} \right) \times (T_i - T) - \frac{k\Delta H_r C_A C_B}{\rho c_p}$$

$T_i$  is the feed temperature, and  $\Delta H_r$  signifies the reaction enthalpy. The reaction enthalpy dictates whether the reaction is endothermic (absorbs heat) or exothermic (releases heat), further influencing reactor temperature dynamics.

With this theoretical foundation, we are equipped to simulate the reactor's behavior under various conditions, thereby unveiling patterns and insights pertinent to reactor operation and design.

## 3. Methodology

The methodology employed for this study revolves around using MATLAB as a simulation tool to investigate the behavior of the CSTR system under different initial conditions. The entire process can be broken down into various sequential steps, which are detailed below:

### 3.1 Description of the MATLAB Approach Used

MATLAB, renowned for its robust numerical solvers and versatile environment, was utilized to simulate the CSTR system dynamics. The system's governing equations, derived from first reaction kinetics and energy balance principles, were solved numerically using the ode113 solver, an adaptive Runge-Kutta method ideal for stiff or non-stiff systems.

### 3.2 Model Setup: Definitions of Constants and Parameters

All relevant parameters and constants were defined to set up the reactor model:

- Feed concentrations: **C\_A0**, **C\_B0**, and **C\_P0**.

- Reactor volume ( $V_R$ ) and volumetric flow rate ( $V_f$ ).
- Activation energy ( $E$ ) and frequency factor ( $A$ ).
- Reaction enthalpy ( $\Delta H_r$ ).
- Heat capacity ( $\rho_{c_p}$ ).
- Universal gas constant ( $R$ ).
- Feed temperature ( $T_0$ ) and system initial temperature ( $T_i$ ).

These parameters form the backbone of the simulations, providing necessary inputs for our differential equations.

### 3.3 ODE Function Description

The core function `odefun` was implemented to contain the differential equations governing the CSTR system's behavior. Within this function:

- The reaction rate constant,  $k$ , was determined using the Arrhenius equation.
- The reaction rate,  $r$ , was computed using the second-order rate law.
- Material balances for components **A**, **B**, and **P** were formulated based on inlet and outlet flow rates and the reaction rate.
- An energy balance was derived considering the adiabatic nature of the reactor, heat introduced via the feed, and heat generated or absorbed due to the reaction.

### 3.4 Simulation Strategy: Varying the Initial Reactor Temperature

To investigate the CSTR dynamics under various conditions, the system's initial temperature,  $T_i$ , was varied in a defined range (from 290 K to 400 K in increments of 10 K). For each iteration, the differential equations were solved over a specified time span using `ode113`. Also, results were plotted to visualize the concentrations of A, B, and P, alongside the reactor temperature as a function of time. The simulation outputs were saved as image and data CSV files for further analysis.

### 3.5 Plotting and Results Interpretation Methods

The results were visualized for each simulation corresponding to a specific initial temperature using MATLAB's plotting functions. Each plot featured:

- Concentrations of components A, B, and P on the primary y-axis.
- Reactor temperature on the secondary y-axis, ensuring clear differentiation.
- Time (in hours) on the x-axis.
- A legend indicating each plotted variable for clarity.
- A grid for easy reference and title indicates the simulation's initial temperature.

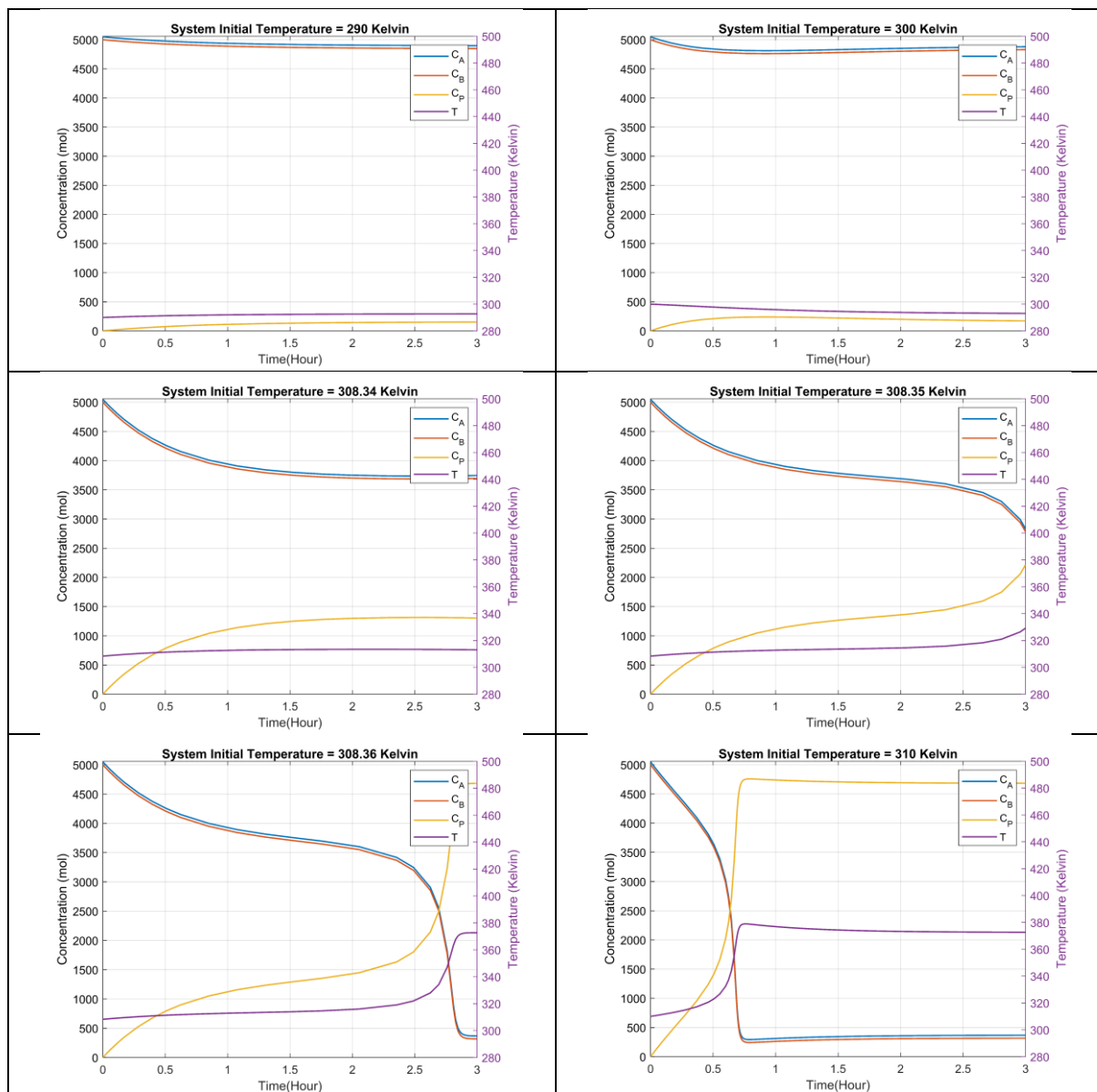
These plots visually represent the CSTR's dynamic response, facilitating insights into how initial temperature influences reactor behavior.

## 4. Results and Discussion

Through the MATLAB simulation, an in-depth analysis of the reactor dynamics was performed by monitoring the variations in concentrations and temperature within the reactor vessel. The objective was to observe the system dynamics until a steady state was achieved.

The reactor was assumed to be initially filled with an inert solvent for our investigation. The initial temperature, denoted as  $T_i$ , was varied in a range of 290-400 K. The goal was to study how this wide temperature span affects the reactor dynamics. Specifically, twelve different simulations were conducted, each differing in its initial reactor temperature.

The feed temperature, denoted as  $T_0$ , remained consistent at 290 K throughout all simulations. The results were plotted in Figure 1 for each specific initial temperature, illustrating concentrations of components A, B and P and temperature.



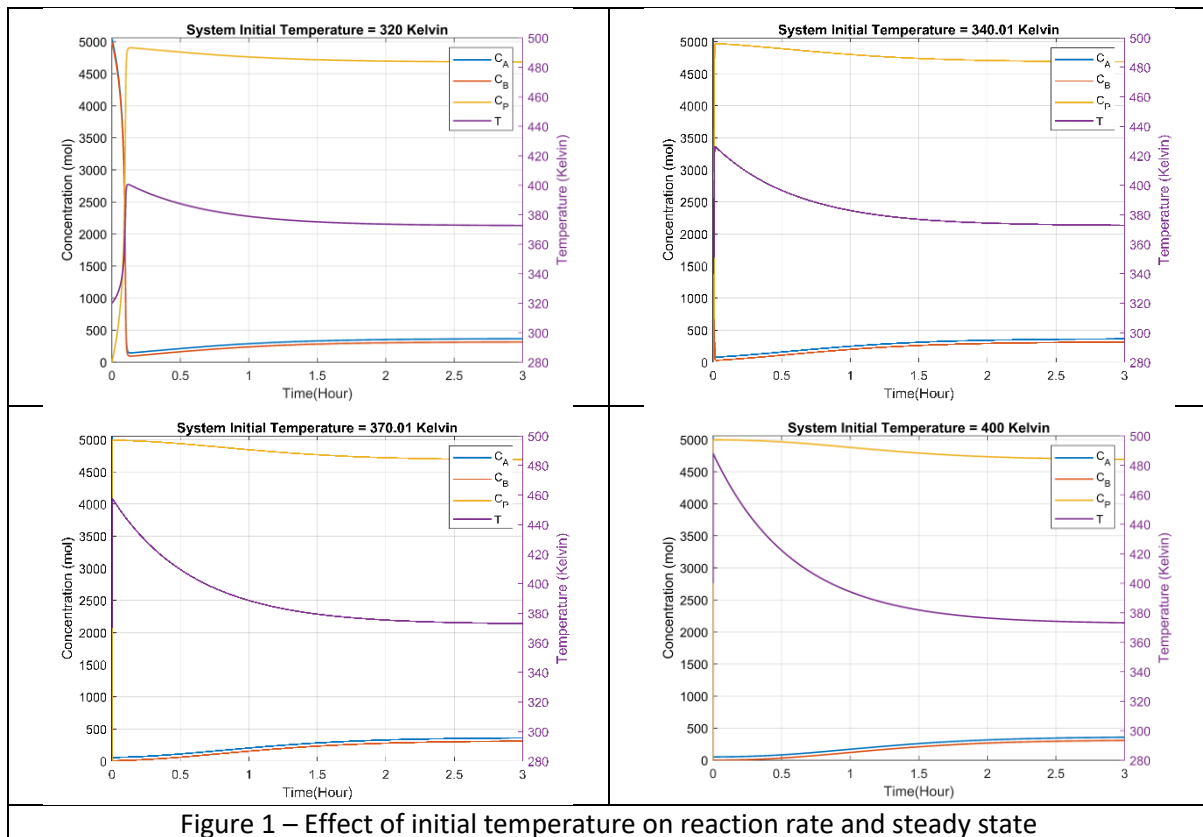


Figure 1 – Effect of initial temperature on reaction rate and steady state

On visual inspection of the plots, the following key observations emerged:

- Typically, an increase in temperature will increase the reaction rate, assuming the reaction is endothermic. This is due to the Arrhenius equation, which shows that the reaction rate constant ( $k$ ) increases with increasing temperature. As  $T_i$  rises, the value of  $k$  would be higher at the beginning of the reaction, leading to a faster initial reaction rate. In the plots generated above, faster reaction rates should correspond to steeper initial slopes for the concentration curves. Also, it shows how the increase in  $T_i$  can lead to multiple steady states.
- Reaching a steady state means the system's variables (concentrations and temperature) no longer change with time. The speed at which a steady state is reached can be affected by  $T_i$ . A higher initial temperature drives the system to its steady state faster.
- Since the reaction is exothermic (releases heat), the reaction will generate its own heat, potentially raising the system's temperature. Starting with a higher  $T_i$  might mean the system reaches a maximum tolerable temperature faster, potentially slowing or stopping the reaction if it gets too high. In the plots, the temperature ( $T$ ) curve plateaus or even decreases after initially increasing, indicating the system reaches a maximum temperature due to the heat of the reaction.
- A faster reaction rate typically means products are formed more quickly. However, the total amount of product formed when the system reaches a steady state might not necessarily change with varying  $T_i$ . The initial temperature affects the speed of product formation but not the final product amount.
- The concentration of product  $P$  demonstrated intriguing behavior. With lower initial temperatures, the production rate gradually showed a standard behavior of reactants

converting to products. However, upon reaching a certain threshold (around  $T_i = 308$  K), there was a pronounced spike in the production of P. This implies that the reaction kinetics were significantly amplified, rapidly converting A and B to P.

- For the temperature dynamics, a clear trend was not always consistent across all simulations. However, a particular attention-grabbing behavior was noted post the threshold of  $T_i = 308$  K, where an initial spike in temperature was observed, possibly due to the exothermic nature of the reaction and the sudden increase in reaction rate.

The initial temperature ( $T_i$ ) can significantly influence the dynamics of a chemical reaction system. It can affect the reaction speed, the time taken to reach a steady state, and the system's overall behavior. Careful control and understanding initial conditions, like temperature, are crucial for optimizing chemical processes and ensuring safety.

## 5. Conclusion

The study provided a comprehensive analysis of the behavior of a Continuous Stirred Tank Reactor (CSTR) system by varying the initial temperature. The findings demonstrate that initial temperature,  $T_i$ , significantly influences the system's dynamics in terms of reaction speed, concentrations of reactants and products over time, and overall temperature profile. The importance of the Arrhenius equation was further solidified by observing the correlation between the initial temperature and the reaction rate. The significance of this study lies in its ability to offer insights crucial to the design and operation of CSTRs. In real-world applications, understanding the influence of initial temperature on system dynamics will aid in optimizing reactor performance, enhancing productivity, and ensuring operational safety. The intriguing observation of multiple steady states under specific conditions underscores the potential challenges and complexities in reactor operation and design.

## 6. Recommendations

Based on the findings and analysis of this study on Continuous Stirred Tank Reactors (CSTRs), the following recommendations are proposed:

1. **Safety Protocols:** As observed in this study, certain initial temperatures led to rapid reaction rates and potential temperature spikes. For industrial-scale reactors, such behaviors could pose safety hazards. It must incorporate safety interlocks and automated shutdown mechanisms to counteract sudden temperature increases.
2. **Advanced Control Systems:** Given the reactor's sensitivity to initial conditions and observing multiple steady states, deploying advanced control strategies, such as adaptive or model predictive control, could be beneficial for maintaining reactor stability and achieving desired product quality.
3. **Integration with Real-time Monitoring:** Implement real-time monitoring systems equipped with robust sensors to track the temperature and concentration profiles inside the reactor continuously. Immediate feedback can be invaluable for on-the-fly adjustments and prompt interventions in case of deviations.
4. **Model Refinement:** Continually refine and update the reactor model based on actual plant data and experiences. Periodic validation of the simulation model with plant data ensures its relevancy and reliability for future studies.

5. **Feedback Loop:** Establish a feedback mechanism where insights from real-world operations are fed back into the research and design phase, ensuring continuous improvement and evolution of reactor designs and operating strategies.

In conclusion, while this study provides significant insights into the behavior of CSTRs under varying initial temperatures, it is vital to view these findings as a starting point. Continual research and practical experiences will ensure safer, more efficient, and more productive CSTR operations.



# Appendices

## (A) MATLAB code

```
clc
clear all
close all
obj.C_A0 = 5050; %mol/m3 Feed concentrations
obj.C_B0 = 5000; %mol/m3 Feed concentrations
obj.C_P0 = 0; %mol/m3 Feed concentrations
obj.V_R = 1.20; %m3 Reactor volume
obj.V_f = 0.6e-3; %m3/s Volumetric flow rate
obj.E = 99000; %J/mol Activation energy
obj.A = 1.52e9; % m3/(mol.s) Frequency factor
obj.deltaH_r=-33.5e3; % Reaction enthalpy
obj.rho__c_p = 1900e3; % J/(m3K) Heat capacity
obj.R = 8.314; %
obj.T0 = 290;%K feed Temperature
obj.Ti = 312; %K System initial Temperature
tspan = [0, 10800]';
loopT = 290.01:10:400.01; %K System initial Temperature (Investigation range)

% loopT = 301.01:1:309.01;
% loopT = 308.1:0.1:309.9;
% loopT = 308.31:0.01:308.39;
for i = 1:length(loopT)
    clear results
    clear fig
    obj.Ti = loopT(i);
    results = ode113(@(t,y) odefun(t, y, obj), tspan, [obj.C_A0, obj.C_B0, obj.C_P0, obj.Ti]);
    results.xH = results.x/3600;
    fig = figure();
    plot(results.xH, results.y(1:3,:), 'LineWidth', 1.2);
    ylabel('Concentration (mol)')
    ylim([0, 5060])
    yyaxis right;
    plot(results.xH, results.y(4,:), 'LineWidth', 1.2);
    ylabel('Temperature (Kelvin)')
    ylim([280, 500])
    legend('C_A', 'C_B', 'C_P', 'T')
    xlabel('Time(Hour)')
    title(['System Initial Temperature = ', num2str(obj.Ti), ' Kelvin'])
    grid on
    print(fig,['T=', num2str(obj.Ti) , '.png'],'-dpng','-r1500');
    writematrix([round(results.x,4); round(results.y,2)]', ['T=', num2str(obj.Ti) , '.csv']);
    % Time, C_A, C_B, C_P, T
    disp(['Calculation for Ti= ', num2str(loopT(i)), '(K) is finished. You can check the results'])
end

function dydt = odefun(t,y, obj)
    C_A = y(1);
    C_B = y(2);
    C_P = y(3);
    T = y(4);
    k = obj.A* exp(- obj.E / (obj.R*T));
    r = k * C_A * C_B;
    dydt(1,1) = obj.V_f / obj.V_R * (obj.C_A0 - C_A) - r;
    dydt(2,1) = obj.V_f / obj.V_R * (obj.C_B0 - C_B) - r;
    dydt(3,1) = obj.V_f / obj.V_R * (obj.C_P0 - C_P) + r;
    dydt(4,1) = (obj.V_f/obj.V_R) * (obj.T0 - T) - (obj.deltaH_r * k * C_A * C_B)/(obj.rho__c_p);
end
```