# DEVELOPING A MATHEMATICAL MODEL OF THE POLYMERIZATION REACTOR BASED ON THE INITIAL DATA SET FOR THE PRODUCTION OF POLYVINYL CHLORIDE

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**Annotation.** In this article, a mathematical model was created in MATLAB based on the heat balance equations of the material balance of the polymerization reactor in the production of polyvinyl chloride.
**Key words:** Database, mathematical model, polymerization reactor, PVC production control system.

**Annotatsiya.** Ushbu maqolada polivinil xlorid ishlab chiqarishda polimerlash reaktorining issiqlik balans material balans tenglamalari asosida MATLAB dasturida matematik model yaratilgan.
**Kalit so'zlar:** Ma'lumotlar bazasi, matematik model, polimerlash reaktori, PVX ishlab chiqarish boshqarish tizimi

**Аннотация.** В данной статье в программе MATLAB создана математическая модель на основе уравнений теплового баланса материального баланса реактора полимеризации при производстве поливинилхлорида.
**Ключевые слова:** База данных, математическая модель, реактор полимеризации, система управления производством ПВХ.

## Introduction

The production of polyvinyl chloride (PVC) is a critical process in the chemical industry, owing to its extensive use in various applications such as construction, healthcare, and consumer goods. PVC is synthesized through the polymerization of vinyl chloride monomer (VCM), a process that requires precise control to ensure the desired quality and properties of the final product. This predictive capability is crucial for improving process efficiency, reducing production costs, and ensuring product consistency. In this article, we focus on the development of a mathematical model for the polymerization reactor used in PVC production. The model is based on an initial data set that includes various operational parameters and chemical properties [1].

## Steps of developing mathematical model of this process.

Creating a mathematical model of the PVC polymerization process in a batch reactor and finding its transfer function involves several steps. Below, I'll outline a general approach and derive the key equations and transfer function [2]

**Step 1: Define the Process and Assumptions**
**Reactants:** Vinyl Chloride Monomer (VCM) and initiator.
**Reactor type:** Batch reactor.
**Key assumptions:**

- The reactor is well-mixed (perfect mixing).



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- Temperature is constant (isothermal conditions).
- The reaction kinetics follow a known rate law.
- The polymerization process is first-order with respect to the initiator and VCM concentrations [3]

**Step 2: Write the Governing Equations**

The polymerization of VCM can be described by the following kinetic equations:

1. Monomer consumption (1):

$$\frac{d[M]}{dt} = -k_p[M][I] \quad (1)$$

where $[M]$ is the monomer concentration, $[I]$ is the initiator concentration, and $kp$ is the rate constant for polymerization [4].

Initiator consumption:

$$\frac{d[I]}{dt} = -k_d[I] \quad (2)$$

where $k_d$ is the rate constant for initiator decomposition.

Polymer production

$$\frac{d[P]}{dt} = k_p[M][I] \quad (3)$$

Where [P] – is the concentration of the polymer

**Step 3: Combine the Equations**

Assuming the initiator concentration is much smaller than the monomer concentration and remains relatively constant (pseudo-steady-state approximation):

$$[I] \approx [I]_0 e^{-kdt}$$

The monomer concentration changes over time as:

$$\frac{d[M]}{dt} = -kp[M][I]_0 e^{-k_d t}$$

If we calculate the integral of this equation over the function [M](t) and exponentiate both sides of the equation, we get the following equation:

$$-[M](t) = [M]_0 \exp\left(-\frac{k_p[I]_0}{k_d}(1 - e^{-k_d t})\right) \quad (4)$$

**Step 4: Transfer Function**

To derive the transfer function, we need to linearize the model around an operating point and apply Laplace transforms [5]

1. **Linearization:**

Let $(t)=M_0+\delta M(t)$ and $I(t)=I_0+\delta I(t)$ Linearize around the steady-state concentrations $M_0$ and $I_0$

**2. Laplace Transform**: Apply Laplace transforms to the linearized equations:

$$\mathfrak{L}\left\{\frac{d\delta M(t)}{dt}\right\} = -k_p \mathfrak{L}\{\delta M(t) I_0 + M_0 \delta I(t)\} \quad (5)$$

Let $\Delta(s)$and $\Delta I(s)$ be the Laplace transforms of $\delta M(t)$and $\delta I(t)$, respectively. The Laplace transform of the above equation is:

$$s\Delta M(s) = -kp(I0\Delta M(s) + M0\Delta I(s))$$

**3.Transfer Function:** Solving for $\Delta M(s)$ in terms of $\Delta I(s)$:

$$\Delta M(s)(s + k_p I_0) = -k_p M_0 \Delta I(s)$$

The transfer function is G(s)= $\Delta M(s)/ \Delta I(s)$:



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$$G(s) = \frac{\Delta[M](s)}{\Delta I(s)} = \frac{k_p M_0}{s + k_p I_0}$$

**Necessary values of parametres**

- Rate constant for polymerization ($k_p$): $2\times10^3$ L/mol
- Rate constant for initiator decomposition ($k_d$): $5\times10^{-4}$ $s^{-1}$
- Initial concentration of monomer ($[M]_0$): 8 mol/L
- Initial concentration of initiator ($[I]_0$): 0.05 mol/L
- Reactor temperature: 60°C
- Reactor volume (V): 5 L

From the previous derivation, the transfer function was:

$$G(s) = \frac{\Delta[M](s)}{\Delta I(s)} = \frac{k_p M_0}{s + k_p I_0}$$

Substituting the values:

$$G(s) = \frac{-2 * 1000 * 8}{s + 2 * 1000 * 0.05} = \frac{-16000}{s + 100}$$

This transfer function describes the dynamic response of the monomer concentration to changes in the initiator concentration for the given set of physical parameters [6]

**Checking mathematical model on MATLAB**

I plot the transient process function of the given transfer function.

```
>> G=tf([-16000],[1 100])

G =

  -16000
  -------
  s + 100

Continuous-time transfer function.

>> step(G)
>>
```

**Fig.1. Code for finding h(t) function**



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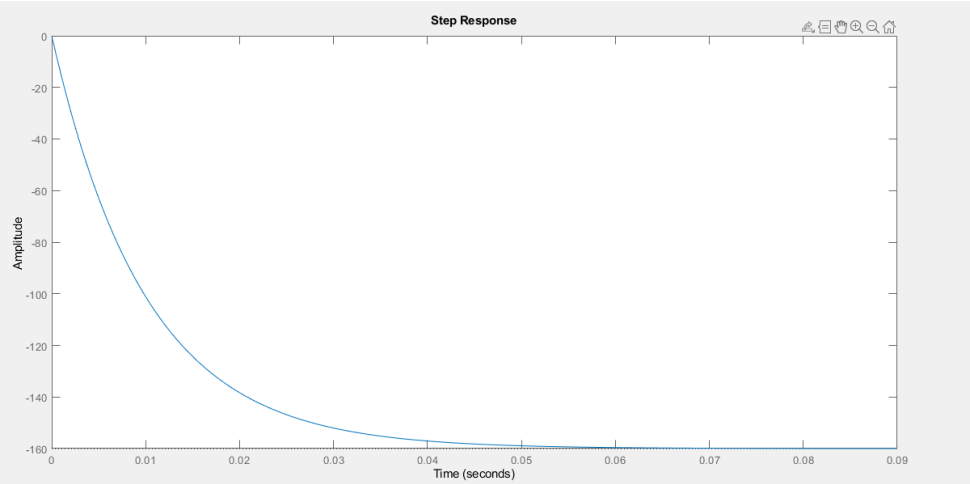


**Fig.2. Step response of transfer function.**

The stability of this system according to the given transfer function is checked by the Nyquist criterion in the MATLAB program.

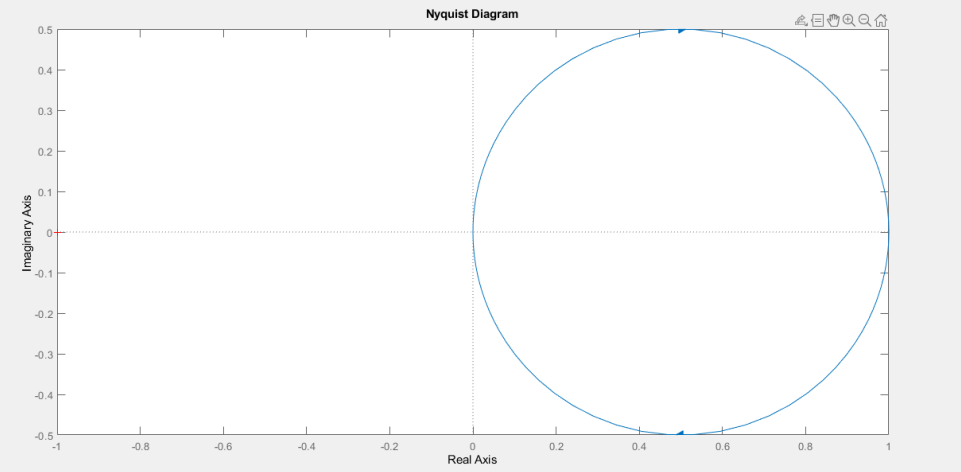


**Fig.3. Amplitude phase characteristic of the transfer function**

Looking at this graph, the mathematical model we have built is stable and has the required quality indicators [7]

## Conclusion

In this study, we have successfully developed a mathematical model of the polymerization reactor for the production of polyvinyl chloride (PVC) based on initial data sets. By leveraging key parameters and reaction kinetics, we have formulated differential equations that describe the dynamic behavior of monomer, initiator, and polymer concentrations within the reactor. The model was implemented and simulated using MATLAB, providing a comprehensive framework for analyzing the polymerization process.

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