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Research Article

Modelling and Simulation of Flow and Level Dynamics in a Pharmaceutical Batch Mixer

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Abstract

A mathematical model and dynamic performance study of a Supervisory Control and Data Acquisition (SCADA) system and a Programmable Logic Controller (PLC) that were previously utilized to automate the pharmaceutical batch mixer are presented in this research. While the earlier work implemented the discrete, sequential control logic for the mixer using Siemens STEP 7 and validated it with RSLogix 5000, the continuous-time hydraulic behaviour of the three interconnected process vessels (heating, mixing and storage tanks) had not been characterised. In this study, the batch mixing system is partitioned into three sections, each represented by a pump-and-tank arrangement, and first-principles mass-balance, Bernoulli energy-balance and Darcy friction-loss equations are used to derive the transfer functions relating pump flow rate and tank level to valve resistance and tank cross-sectional area. Laplace transformation of the governing equations yields an overall block-diagram model of the three-tank system, which is implemented and simulated in MATLAB/SIMULINK. The simulation results show that the flow response settles at 0.5 m3/s with a settling time of 1.32 x 10^4 seconds, an overshoot of 11.5% and a rise time of 4.03 x 10^3 seconds. The tank-level responses show a successive filling pattern consistent with the batching sequence, with Tank 1 filling within 20 minutes, Tank 2 reaching its maximum level at 65 minutes, and Tank 3 completing filling at 210 minutes from the start of the process. These results confirm that the batch mixer exhibits stable, well-damped dynamic behaviour, providing a quantitative basis for the timer presets and control logic used in the PLC-SCADA automation reported previously, and supporting the suitability of the process for closed-loop SCADA-based control.

Keywords

Batch Mixer, Mathematical Modelling, Transfer Function, MATLAB/SIMULINK, Performance Analysis, Programmable Logic Controller, Supervisory Control and Data Acquisition, Pharmaceutical Process

1. Introduction

In the food, chemical, and pharmaceutical industries, automating batch processes boosts production throughput, decreases human error, and enhances product uniformity, [2, 3] [5]. An automated system for a mixing process that might be used in oil refineries, the food, chemical, pharmaceutical, and process sectors. A Programmable Logic Controller governs the entire proposed system (PLC). The MicroLogix 500 Rock-

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well Automation software is programmed using ladder diagrams, which are incredibly intuitive and easy to understand. The system automatically blends the solutions from two different tanks, batch by batch, in the third tank with the help of a stirrer [4-6]. With a focus on temperature control utilizing a cooling jacket under perfect mixing, two significant reactors, batch and non-isothermal CSTR, were studied. MATLAB and ASPEN PLUS simulations are used to examine reactor behavior during exothermic processes. Within the software, the ASPEN PLUS simulation adheres to a defined process. The approach generally improves the design and optimization of industrial chemical processes by combining theory and simulation [7, 9, 10].

In a study, a mathematical model for the oxidative desulfurization of kerosene was created. The model's estimation of kinetic parameters is based on experimental data found in the literature. gPROMS software was used for simulation and optimization. Ea = 18.64 kJ/mol, pre-exponential factor = 2201.34, and reaction order = 1.77 were the ideal kinetic constants. For ≥99 percent conversion, these values provided ideal conditions of 379.4 K and 160 min. The ideal batch reactor diameter, according to scale-up studies, is 1.2 m [8]. In a previous study, the authors described automating a manually operated pharmaceutical batch mixer by integrating a Supervisory Control and Data Acquisition (SCADA) Human Machine Interface (HMI) built in InTouch Wonderware with a Programmable Logic Controller (PLC) programmed in Siemens STEP 7 ladder logic [1] This work used Rockwell Automation's RS Logix 5000 software to cross-check the ladder logic and implement and validate the discrete, event- and time-driven control sequence that governs the mixer's heating, blending, draining, and storage phases.

The nominal step durations for each stage of the process (such as a 45-minute reaction period, a 60-minute blending period, and a 45-minute drain period) specified in the PLC-SCADA implementation in [1] were primarily determined from process requirements rather than an examination of the underlying hydraulic dynamics of the mixer vessels. Therefore, to determine whether these nominal timings are consistent with the system's physical response and to provide a foundation for future closed-loop or model-based control of the mixer, a quantitative, first-principles characterization of the plant's flow and level dynamics is required.

In order to close that gap, this paper develops a mathematical model of the three interconnected process vessels of the batch mixer using mass-balance, energy-balance, and valve-restriction equations. It then derives the corresponding transfer functions and uses MATLAB/SIMULINK simulation to validate the resulting dynamic behavior. The rest of the paper is structured as follows: The batch mixer's mathematical modeling and simulation are presented in Section 2; the results are shown in Section 3; the findings are discussed in relation to the PLC-SCADA implementation published in [1] and other related work in Section 4; and the study is concluded in Section 5.

2. Materials and Methods

A lumped-parameter, first-principles method was used to describe the hydraulic dynamics of the batch mixer. The heating, mixing, and storing vessels mentioned in [1] were represented by the three parts of the plant, each of which had a tank and a corresponding pump. The transfer functions connecting flow rate and tank level to pump and valve parameters were obtained by Laplace transformation by combining the mass-balance, Bernoulli energy-balance, and Darcy friction-loss equations with the valve-restriction connection. The flow and level responses of the three-tank system were simulated to assess settling time, overshoot, and rising time. The resulting model was implemented in MATLAB/SIMULINK using the parameter values summarized in Table 1.

2.1. Mathematical Modelling

Figure 1 shows the system that has to be modeled. Figures 4 and 5 illustrate the reorganization of the batch mixer system modeling into three pieces.

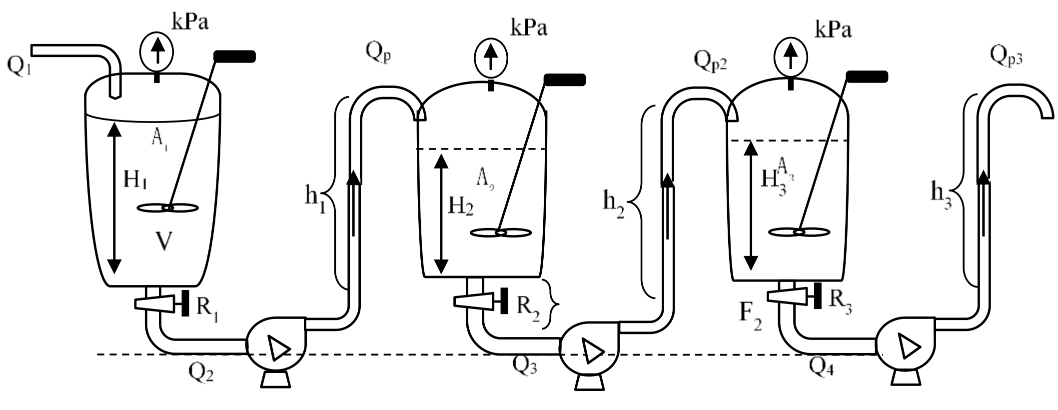

Figure 1. *Modeling of a Batch Mixing System.*

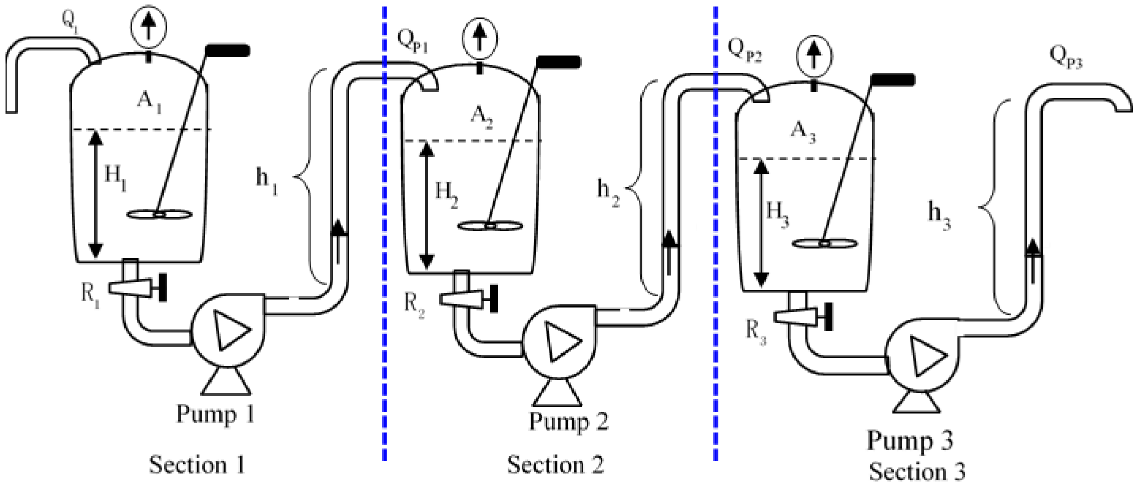

Figure 2. *Sectionalizing the Batch Mixing System for Modelling.*

For the modelling, the following equations were utilized [2, 3, 11, 12, 15]: Equations (1) and (2) represent the mass flow balance equations; Equation (3) represents Bernoulli's energy balance equation; Equation (4) provides the pump's efficiency; Equation (5) provides the volumetric flow rate through a pump; and Equation (6) represents the work performed by the pump and Equation (7) is Darcy's equation which expresses the frictional head loss (caused by e.g. friction, valve expansion and bends) through the pipe [16].

$$m'_i = m'_e + \frac{dM}{dt} \tag{1}$$

$$Q_i = Q_{i+1} + A_i \frac{dH_i}{dt} \tag{2}$$

$$P_i + \rho g h_i + \frac{1}{2}\rho V_i^2 + h_A - h_E - h_L = P_{i+1} + \rho g h_{i+1} + \frac{1}{2}\rho V_{i+1}^2 \tag{3}$$

$$\eta_i = \frac{P_{i\ out}}{P_{input}} \tag{4}$$

$$Q_{Pi} = \frac{P_{i\ out}}{h_A \gamma} \tag{5}$$

$$h_A = \frac{P_2 - P_1}{\gamma} + \frac{V_2^2 - V_1^2}{2g} + h_L \tag{6}$$

$$h_L = \frac{\Delta P}{\gamma} = \frac{P_1 - P_2}{\gamma} = \left(\frac{4\tau_w}{\rho g}\right)\left(\frac{L}{D}\right) = f\left(\frac{L}{D}\right)\left(\frac{V^2}{2g}\right) \tag{7}$$

The restriction of flow by the valve is given by Equation (8) [3].

$$R_i = \frac{H_i(t) - H_{i+1}(t)}{Q_i} \tag{8}$$

Laplace transforms applied to the volumetric flow rate and the restrictions of the valve are given by Equation (9) and Equation (10) respectively.

$$Q_i(s) = Q_{i+1}(s) + A_i s H_i(s) \tag{9}$$

$$Q_i(s) = \frac{H_i(s) - H_{i+1}(s)}{R_i} \tag{10}$$

The system transfer function is obtained in equation (11) by substituting Equation (9) into Equation (10).

$$\frac{Q_{i+1}(s)}{Q_i(s)} = \frac{G(s)}{1+G(s)H(s)} = \frac{1}{A_{i+1}R_{i+1}s+1} \tag{11}$$

where, m_i' initial mass flow rate, kg/s = volumetric flow rate ρQ_i, (m^3/s)

m_e' = mass flow rate at exit, kg/s= volumetric flow rate ρQ_{i+1}, (m^3/s)

M = mass of the system, kg/s = volumetric flow rate $\rho A_i H_i$, (m^3/s)

γ = particular weight of the fluid flowing through the pipe, (dimensionless quantity)

h_A = pump work done, (m)

h_E = loss as a result of extraction (e.g. turbine and windmill) = 0, (m)

h_L = frictional head loss via pipes (such as expansion, bends, valves, and friction) (m)

V_1 and V_2 = velocity upon entry and departure, (m/s)

η = pump efficiency P_1, (no unit)

P_{iout} = flow power that the pump delivers, (Watts)

P_{input} = power input by the motor. (Watts)

Q_{Pi} = volumetric flow rate of pump (m^3/s)

f = frictional factor, (no units)

L = pipe's length, (m)

D = pipe's inner diameter, (m)

P_1 and P_2 = pressure at the pipe's inlet and outlet, (Pa, N/m^2)

v = average speed (m/s)

g = acceleration due to gravity (m/s^2)

ρ = fluid's density, (kg/m^3)

G = the system's gain (dimensionless)

H = gain in feedback (dimensionless)

R = resistance of the valve, (sec/m^2)

τ_i = time constant, (sec)

H_i= height of the tank (m)

A_i = area of tank (m^2)

h_i = height of pipe (m)

τ_w = wall shear stress (Pa)

The three portions are then subjected to Equations (1) through (11) which are first principle methods [9, 10].

2.1.1. Transfer Function for Flow Rate of Syrup Through the Pipe

The volumetric flow rate Q_1, Q_{P1}, Q_{P2} through Pump 1, Pump 2, and Pump 3 are given by Equation (12), (13) and Equation (14).

$$Q_1 = Q_{P1} + A_1 \frac{dH_1}{dt} \quad (12)$$

$$Q_{P1} = Q_{P2} + A_2 \frac{dH_2}{dt} \quad (13)$$

$$Q_{P2} = Q_{P3} + A_3 \frac{dH_3}{dt} \quad (14)$$

Adding Equation (12), (13), and (14) together results in Equation (15) which gives the input flow, Q_1 of sugar crystals to the output flow, Q_{P3} as total flow of the syrup from Tank 1 to Tank 3.

$$Q_1 = Q_{p3} + \left(A_3 \frac{dH_3}{dt} + A_2 \frac{dH_2}{dt} + A_1 \frac{dH_1}{dt} \right) \quad (15)$$

The transfer function of the three sections of the modelled system in Section 1 is given by Equation (16), Equation (17) and Equation (18) respectively [10, 13],

$$\frac{Q_{P1}(s)}{Q_1(s)} = \left(\frac{1}{A_1 R_1 s + 1} \right) \quad (16)$$

$$\frac{Q_{P2}(s)}{Q_{P1}(s)} = \left(\frac{1}{A_2 R_2 s + 1} \right) \quad (17)$$

$$\frac{Q_{P3}(s)}{Q_{P2}(s)} = \left(\frac{1}{A_3 R_3 s + 1} \right) \quad (18)$$

The overall transfer function is given by Equation (19) and Figure 3 summarises the 3-tank system in block diagram form.

$$\frac{Q_{P3}(s)}{Q_1(s)} = \left(\frac{1}{A_3 R_3 s + 1} \right)\left(\frac{1}{A_2 R_2 s + 1} \right)\left(\frac{1}{A_1 R_1 s + 1} \right) \quad (19)$$

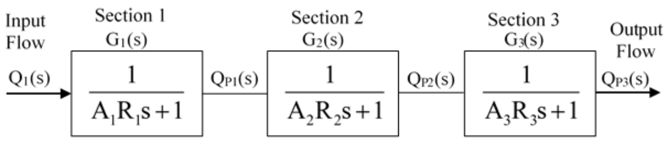

***Figure 3**. Block Diagram of the 3-Tank System.*

Let time constant $\tau_i = A_i R_i$ and Equation (19) results into Equation (20)

$$\therefore \frac{Q_{P3}(s)}{Q_1(s)} = \left(\frac{1}{\tau_3 s + 1} \right)\left(\frac{1}{\tau_2 s + 1} \right)\left(\frac{1}{\tau_1 s + 1} \right) \quad (20)$$

For a unity feedback, the transfer function of Equation (20) results in Equation (21) and finally into Equation (22).

$$\frac{Q_{P3}(s)}{Q_1(s)} = \frac{\frac{1}{(\tau_3 s + 1)(\tau_2 s + 1)(\tau_1 s + 1)}}{1 + \left(\frac{1}{(\tau_3 s + 1)(\tau_2 s + 1)(\tau_1 s + 1)} \right)} \quad (21)$$

$$\frac{Q_{P3}(s)}{Q_1(s)} = \left(\frac{1}{(\tau_1\tau_2\tau_3)s^3 + (\tau_1\tau_2 + \tau_1\tau_3 + \tau_2\tau_3)s^2 + (\tau_1 + \tau_2 + \tau_3)s + 2} \right) \quad (22)$$

2.1.2. Transfer Function of Level of Syrup in the Tank

The volumetric flow rate Q_{Pi} with respect to valve resistance, R_i [10, 13] of the three pumps P_1, P_2, P_3 is given by Equation (23).

$$\left. \begin{aligned} Q_{P1} &= \frac{H_1(t) - H_2(t)}{R_1} \\ Q_{P2} &= \frac{H_2(t) - H_3(t)}{R_2} \\ Q_{P3} &= \frac{H_3(t)}{R_3} \end{aligned} \right\} \quad (23)$$

Substituting for Q_{P1}, Q_{P2} and Q_{P3} in Equation (12), (13), and (14) making use of Equation (23) and rearranging, result in Equation (24), Equation (25) and Equation (26) respectively, which give the input flow rate, Q_1 of sugar crystals to the individual tank levels, H_1, H_2 and H_3.

$$A_1 \frac{dH_1}{dt} = Q_1 - \frac{H_1(t) - H_2(t)}{R_1} \tag{24}$$

$$A_2 \frac{dH_2}{dt} = \frac{H_1(t) - H_2(t)}{R_1} - \frac{H_2(t) - H_3(t)}{R_2} \tag{25}$$

$$A_3 \frac{dH_3}{dt} = \frac{H_2(t) - H_3(t)}{R_2} - \frac{H_3(t)}{R_3} \tag{26}$$

Taking Laplace transforms on both sides of Equation (24), (25) and Equation (26) results in Equation (27), Equation (28) and Equation (29) respectively.

$$H_1(s)(R_1A_1s + 1) - H_2(s) = R_1Q_1(s) \tag{27}$$

$$H_2(s)\left(R_2A_2s + \frac{R_1+R_2}{R_2}\right) - \frac{R_1}{R_2}H_3(s) = H_1(s) \tag{28}$$

$$H_3(s)\left(R_2A_3s + \frac{R_2}{R_3} + 1\right) = H_2(s) \tag{29}$$

Combining Equations (27), (28) and (29) together results in the transfer function of the tank system and presented in Equation (30) then further refined through Equation (31), (32) and finally to Equation (33).

$$\frac{H_3(s)}{Q_i(s)} = \frac{R_1}{\left((\tau_1 s + 1)\left(\tau_2R_2A_3s^2 + \left(R_1A_3 + R_2A_3 + \tau_2 + \frac{R_2}{R_3}\tau_2\right)s + \frac{R_2}{R_3} + \frac{R_1}{R_3} + 1 \right) - \left(R_2A_3s + \frac{R_2}{R_3} + 1\right) \right)} \tag{30}$$

$$\frac{H_3(s)}{Q_i(s)} = \frac{R_1}{\left(\tau_1\tau_2A_3R_2s^3 + \left(\frac{R_2}{R_3}\tau_1\tau_2 + \tau_1\tau_2 + A_3R_1\tau_1 + A_3R_2\tau_1 + A_3R_2\tau_2\right)s^2 + \left(\frac{\tau_1R_1+\tau_1R_2}{R_3} + \frac{R_2}{R_3}\tau_2 + A_3R_1 + \tau_1 + \tau_2 + A_3R_2\right)s + \frac{R_1+R_2}{R_3} + 1 - A_3R_2s - \frac{R_2}{R_3} - 1 \right)} \tag{31}$$

$$\frac{H_3(s)}{Q_i(s)} = \frac{R_1}{\left(\tau_1\tau_2\tau_3R_2s^3 + \left(\frac{R_2}{R_3}\tau_1\tau_2 + \tau_1\tau_2 + \tau_1A_3R_1 + \tau_1A_3R_2 + \tau_2\tau_3R_2\right)s^2 + \left(\frac{\tau_1R_1}{R_3} + \frac{\tau_1R_2}{R3} + \frac{\tau_2R_2}{R3} + A_3R_1 + \tau_1 + \tau_2\right)s + \frac{R_1}{R_3} \right)} \tag{32}$$

Multiply numerator and denominator by R_3 and designate $R_3A_3 = \tau_3$

$$\frac{H_3(s)}{Q_i(s)} = \frac{R_1R_3}{\left(\tau_1\tau_2\tau_3R_2s^3 + (\tau_1\tau_2 + \tau_1\tau_3R_3 + \tau_1\tau_3R_1 + \tau_1\tau_3R_2 + \tau_2\tau_3R_2)s^2 + (\tau_1R_1 + \tau_1R_2 + \tau_2R_2 + \tau_3R_1 + \tau_1R_3 + \tau_2R_1)s + R_1 \right)} \tag{33}$$

Table 1. *Parameter Values for Three Tanks System.*

Parameter	Value	Unit
A_1	24.22	m^2
A_2	24.22	m^2
A_3	24.22	m^2
R_1	49	m^2/sec
R_2	107.5	m^2/sec
R_3	107.5	m^2/sec
H_1	1.5	m
H_2	3.5	m
H_3	3.5	m

Simulation results

The behavior of the three-tank liquid flow and level control system was simulated and analyzed using the MATLAB/SIMULINK software package [10, 12, 14]. The outcomes of the step-by-step simulations are displayed in Figures (4), (5), and (6), respectively.

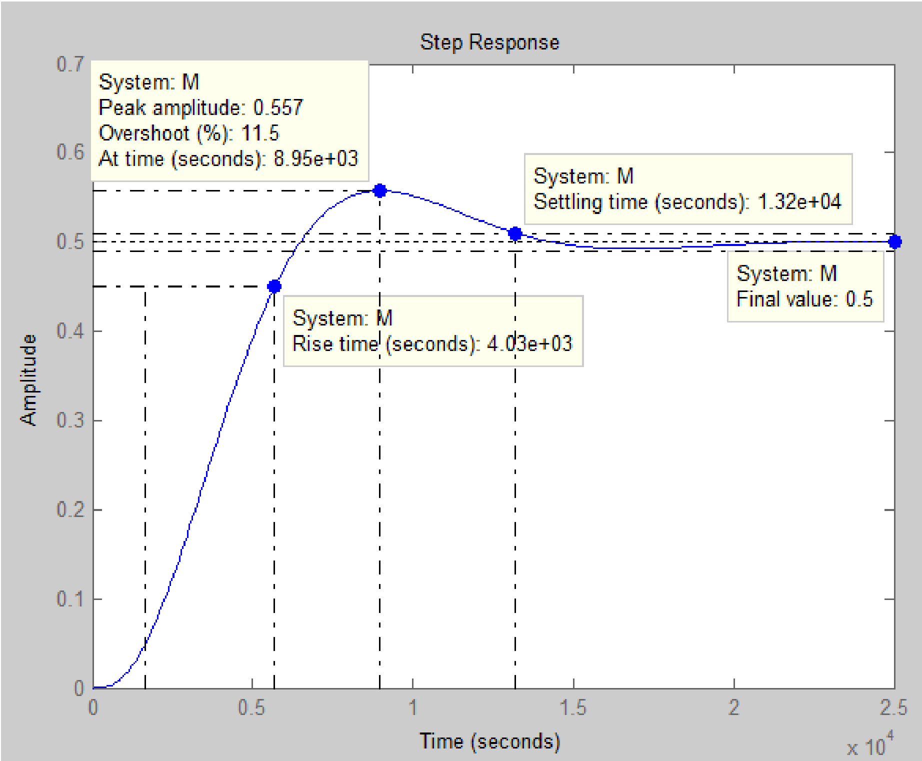

Figure 4. *Step Response of Flow for the Three Tanks.*

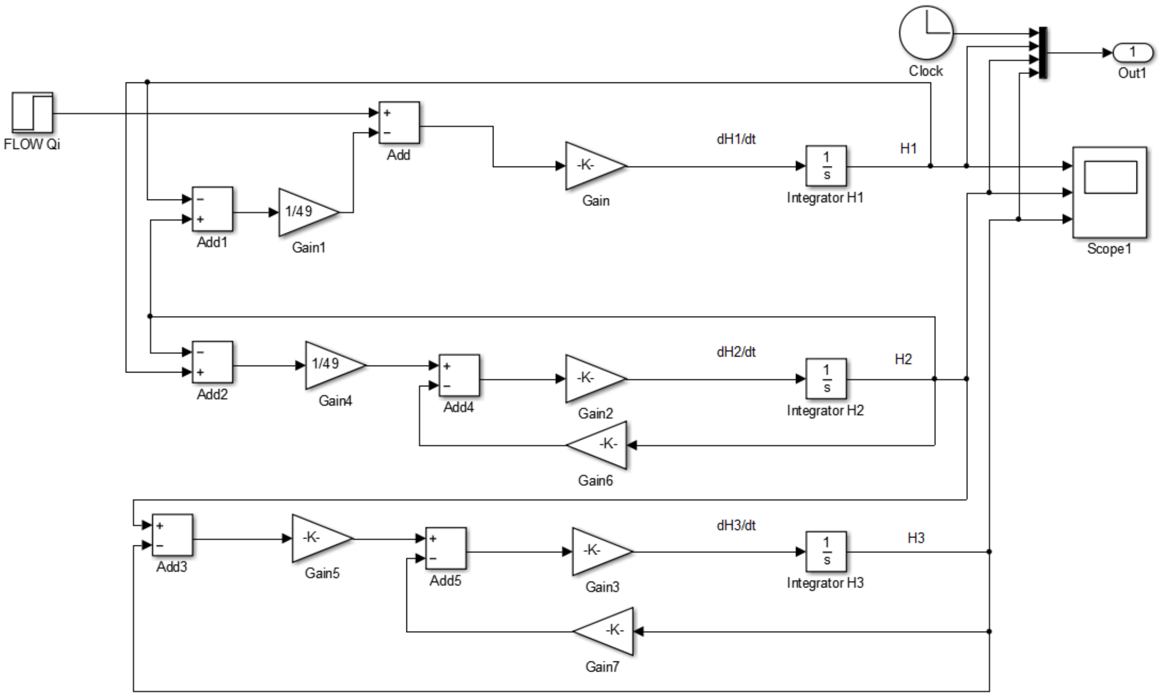

Figure 5. *Simulink Representation for Level of Tanks of the System.*

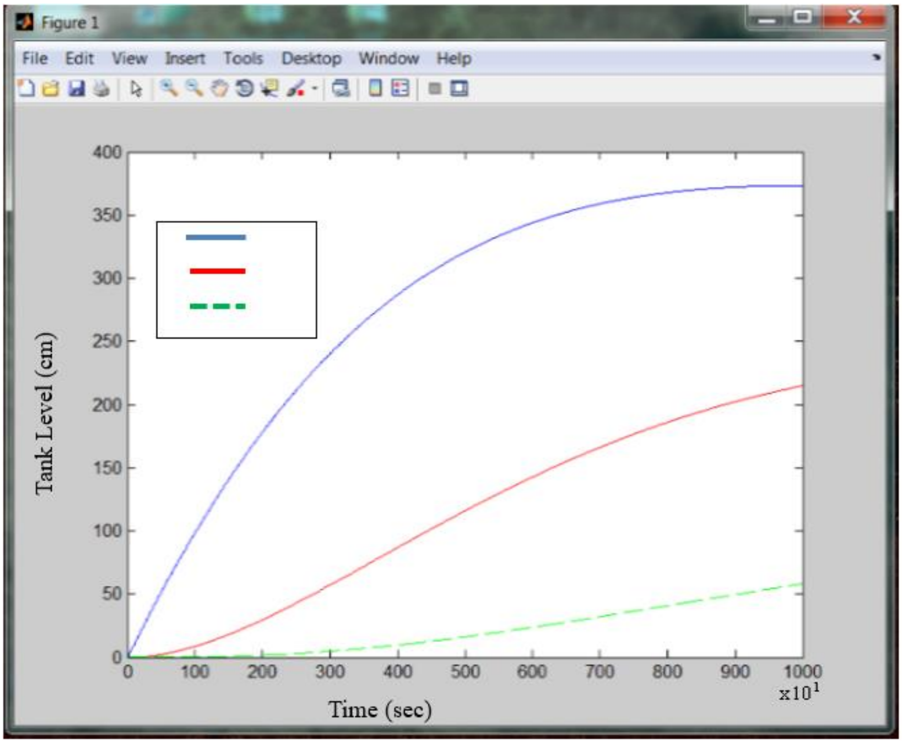

Figure 6. *Output Level Responses of Tank with Respect to Time.*

2.2. System Response to Syrup Flow and Tank Level Dynamics

The way the system behaves in relation to flow of syrup and tank level went normal as expected. For flow looking at Figure 4, the system settles to 0.5 m^3/s for a settling time of 1.32×104 seconds following an 11.5% overshoot [10, 14]. The rise time achieved was 4.03×10^3 seconds. Tank levels, as could be seen from Figure 6 show that the tanks fill up successively i.e. Tank 1 fills in 20 mins after which Tank 2 begins to fill and maximizes its level at 65 minutes from start. Tank 3 fills up after 210 minutes from start of filling. System behavior with regard to flow and level promises good stability. The system therefore can lend itself to SCADA automation making use of PLC and required sensors and transducers.

3. Results

The transfer-function model of the three-tank batch mixer system, derived in Section 2.1, was implemented in MATLAB/SIMULINK using the parameter values in Table 1. The flow-rate step response (Figure 4) settles at 0.5 m3/s with a settling time of 1.32 x 10^4 seconds, an overshoot of 11.5% and a rise time of 4.03 x 10^3 seconds, indicating an underdamped but stable response with a moderate transient before reaching steady state. The tank-level responses (Figure 6) confirm the expected successive-filling behaviour of the three-section arrangement: Tank 1 (heating vessel) fills within 20 minutes, Tank 2 (mixing vessel) reaches its maximum level at 65 minutes from the start, and Tank 3 (storage vessel) completes filling at 210 minutes from the start of the process. This sequential level progression mirrors the staged process described in the nominal batch statement list of the automated system [1], in which the heating, blending and draining operations proceed one after another rather than concurrently. No instability, oscillatory divergence or excessive overshoot was observed in either the flow or level responses across the simulated range, indicating that the plant dynamics are well within the bounds required for reliable PLC-SCADA supervision and control.

4. Discussion

The dynamic model developed in this study complements the discrete-event automation reported in [1]. Whereas the earlier work established that the mixer's heating, blending, draining and storage stages could be reliably sequenced and monitored through PLC ladder logic and a SCADA HMI, it did not quantify the underlying hydraulic response of the plant. The present analysis shows that the settling and rise times of the flow response, and the successive tank-filling times obtained from simulation, are broadly consistent with the nominal step durations used in the PLC program in [1] (for example, the multi-tens-of-minutes duration allotted to each stage), suggesting that the timer presets selected for the automated sequence are compatible with the plant's physical response rather than arbitrary. Compared with related studies that model tank-based process dynamics, such as the two-tank level control system of Fellani and Gabaj [3] and the flow-tank modelling of Jagnade et al. [2], the present model extends the analysis to a three-section, pump-coupled arrangement representative of an industrial batch mixer rather than a single isolated tank, and integrates the resulting transfer functions into a single block-diagram representation suitable for future controller design. The model, however, is a linearised, lumped-parameter representation that does not capture the thermal dynamics of the heating stage or possible nonlinearities in valve behaviour; it also does not include disturbance or noise inputs. Future work should extend the model to incorporate the temperature dynamics of the heating vessel documented in [1] and use the derived transfer functions as the basis for closed-loop PID or model-based control design, building on the open-loop PLC-SCADA sequencing already implemented.

5. Conclusions

A mathematical model of the pharmaceutical batch mixer's three interconnected process vessels was developed from mass-balance, energy-balance and valve-restriction relationships, and the corresponding transfer functions were derived through Laplace transformation. Simulation of the resulting block-diagram model in MATLAB/SIMULINK showed that the flow response settles at 0.5 m3/s with a settling time of 1.32 x 10^4 seconds and an overshoot of 11.5%, and that the tank levels fill successively within the process, from 20 minutes for the first vessel to 210 minutes for the final vessel. These results demonstrate that the batch mixer possesses stable, well-damped dynamic behaviour. Taken together with the PLC-SCADA automation of the same system previously reported, this performance analysis provides a quantitative basis for the timing and control parameters used in the automated sequence, and lays the groundwork for future closed-loop control of the batch mixing process.

Abbreviations

SCADA	Supervisory Control and Data Acquisition System
PLC	Programmable Logic Controller
HMI	Human Machine Interface

Author Contributions

Augustine Kweku Mbeah: Conceptualization, Formal Analysis, Methodology, Software, Writing – original draft

Erwin Normanyo: Methodology, Supervision, Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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Research Field

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