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Conceptual Design of a Mixing System in Alcohol-Based Handrub Production

Delgado-Delgado, R.
Area of basic sciences and engineering
Autonomous University of Nayarit
Tepic, Nayarit, México

Hidalgo-Millán, A.
Area of basic sciences and engineering
Autonomous University of Nayarit
Tepic, Nayarit, México

Rodríguez-Rivera, A. E.
Area of basic sciences and engineering
Autonomous University of Nayarit
Tepic, Nayarit, México

Rodríguez-Lazcano, Y.
Area of basic sciences and engineering
Autonomous University of Nayarit
Tepic, Nayarit, México

ABSTRACT
Mixing is a fundamental operation in the chemical process industry, ensuring homogeneity, facilitating mass and heat transfer, and meeting product specifications. This study presents the conceptual design of a stirred mixing tank for the production of alcohol-based handrub, in alignment with World Health Organization standards. The system incorporates four feed solutions—ethanol, hydrogen peroxide, glycerol, and water—whose mass fractions were determined using Aspen Plus® simulations. A dynamic model was developed and simplified to a steady-state model, resulting in a system of ten linear and nonlinear equations. Degrees of freedom analysis identified 16 design variables, including feed compositions, outlet flow rate, and selected mass fractions. The nominal design achieved a production rate of 100 kg/h, with an ethanol concentration of 75.65% (w/w) in the final product, complying with World Health Organization specifications. The resulting tank dimensions were 0.48 m in both diameter and liquid height, corresponding to a working volume of 0.087 cubic meters. These results establish a framework for detailed studies on operating conditions, control schemes, and process optimization of stirred tank systems used in the large-scale production of alcohol-based handrub formulations.

***Keywords* — handrub; mixing tank; conceptual design; mathematical model**

I. INTRODUCTION

Mixing is a fundamental unit operation in the chemical process industry, which involves combining two or more components (solids, liquids, or gases) to produce a homogeneous or heterogeneous mixture with the desired properties. This process seeks to ensure uniform distribution of materials, whether to facilitate chemical reactions, improve heat or mass transfer, or meet product specifications [1], [2], [3].

The design of mixing systems is a complex engineering discipline that depends fundamentally on the properties of the components and the desired outcome. First, fundamental principles, such as material and energy balances, are applied to define the scope and requirements of the system. This basic step ensures mass conservation and determines the precise quantities of inputs and outputs. In addition, key parameters include fluid rheology (Newtonian or non-Newtonian), density and particle size distribution of solids, and interfacial tension between immiscible liquids. Engineers must select the appropriate agitator type (e.g., turbines, propellers, or high-shear impellers), tank geometry, baffle configuration, and operating conditions to achieve the required mixing intensity [4], [5], [6].

Mixing operations can be performed in either batch or continuous processes. In batch mixing, all components are charged into a vessel and mixed for a defined period until homogeneity is achieved; this method provides high flexibility and is ideal for small-scale production or multi-product facilities. In contrast, the continuous mixing process involves a sustained feed flow of raw materials into a mixer (such as an in-line static mixer or a continuous agitated tank) with simultaneous product withdrawal. This mode of operation is well-suited for continuous manufacturing and high-volume production, and is often integrated with other continuous unit operations within industrial plants [7], [8], [9].

Applications of mixing are broadly utilized across industries. In the chemical sector, it is essential for producing paints, coatings, adhesives, and polymers, where the dispersion of pigments and fillers determines product quality. In the food and pharmaceuticals industries, mixing ensures the uniform distribution of active ingredients, flavors, and vitamins. Specifically, in the production of cleaning products like disinfectants and detergents, mixing is crucial for blending surfactants, solvents, and fragrances. A representative example is the manufacturing of antibacterial liquid, such as hand sanitizer or handrubs, where the precise and homogeneous combination of alcohols, gelling agents, emollients, and water is vital for both efficacy and user safety [10], [11], [12].

The importance of antibacterial liquid reached high levels during the COVID-19 pandemic. Its widespread use was one of the main public health strategies. Demand reached unprecedented levels, highlighting its fundamental role in infection control. The World Health Organization (WHO) emphasized its use for hand hygiene when soap and water are not available. The surge in demand had an immediate impact on production growth, while maintaining strict adherence to

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formulations that ensure the effective inactivation of pathogens, underscoring the vital link between reliable mixing processes and global health security [13], [14], [15].

The manufacturing of effective antibacterial solutions, particularly alcohol-based hand rubs (ABHRs), requires a meticulously controlled process to guarantee microbiocidal efficacy and regulatory compliance. The formulation, primarily comprising isopropyl or ethanol alcohol, must be homogenized with excipients such as glycerin and, in some cases, a thickening agent in a specific sequence to prevent issues like polymer coagulation or alcohol volatilization. This process is crucial for achieving a uniform distribution of the active ingredient, ensuring every aliquot contains the correct alcohol concentration (60-95%) to inactivate pathogens effectively. Furthermore, the equipment must adhere to stringent sanitary standards (e.g., ASME BPE), utilizing closed vessels and mixers capable of handling a wide viscosity range to maintain product sterility, stability, and ultimately, public health safety [15], [16], [17], [18].

The aim of this work is to model and design conceptually a mixer system for the production of alcohol-based handrub in accordance with the quality standards established by WHO, [15]. This contribution highlights the importance of mixing in the production of healthcare products. It provides a foundation for detailed engineering, as well as for studies on the operation and control of the mixing processes.

II. METHODOLOGY

A. Chemical components of the mixing system

The chemical components used in the production of alcohol-based handrub were ethanol, water, glycerol, and hydrogen peroxide. Four different solutions were employed to feed the mixing tank, as shown in Table 1. The composition of the four feed streams was converted from volume fraction to mass fraction using pure component densities from the Aspen Plus ® simulator.

B. Target product specifications

The product stream from the mixing tank is an antibacterial liquid solution (handrub), whose chemical composition is 80% (v/v) ethanol, 1.45% (v/v) glycerol, 0.125% (v/v) hydrogen peroxide, and the remainder water, as per WHO, [15]. Furthermore, a production rate of 100 kg/h was selected as the design basis for the product.

The volumetric composition of the product stream was converted to a mass fraction basis using pure-component density data predicted by the Aspen Plus® simulator.

TABLE 1. FEED SOLUTIONS SUPPLIED TO THE MIXING TANK FOR THE PRODUCTION OF ALCOHOL-BASED HANDRUB.

Component	**Solution 1**	**Solution 2**	**Solution 3**	**Solution 4**
	Volume fraction	***Volume fraction***	***Volume fraction***	***Volume fraction***
Ethanol	0.96	0	0	0
Water	0.04	0.97	0.02	1
Glycerol	0	0	0.98	0
Hydrogen peroxide	0	0.03	0	0

C. Mathematical modeling

The mathematical model of the mixing tank was developed using systematic procedures [19], [20]. The term for the mass of the system in the mass balance equations of the mathematical model was expressed as a function of its volume and density.

On the other hand, the mixing tank was assumed to have a cylindrical geometry, allowing the liquid holdup to be formulated in terms of the liquid height and the cross-sectional area of the tank. Additionally, a 3/8-inch stainless steel solenoid valve (Burkert®) was selected for the tank outlet to achieve the desired flow rate of the product stream. The solenoid valve exhibits a flow coefficient of 0.54 $m^3/h\ bar^{1/2}$ at full opening.

III. RESULTS AND DISCUTIONS

A. Mixing tank feed streams

Based on the data in Table 1, the compositions of the feed streams and final product were determined in terms of mass fraction, as shown in Table 2. The calculations were performed using the Aspen Plus® simulator (AspenTech, 2017), considering the densities of the components at standard pressure and temperature conditions (1 atm and 60 °F). Solutions 1-4 represent the feed streams of the mixing tank, whereas solution 5 corresponds to the alcohol-based handrub product stream. Specifically, solution 1 exhibits an ethanol concentration of 95.01% (w/w). In contrast, the product stream (solution 5) presents an ethanol concentration of 75.65% (w/w), which meets the established requirements of WHO, [15].

The volume of liquids varies with temperature due to thermal expansion and molecular interactions during mixing; therefore, it is appropriate to express the system on a mass basis rather than a volumetric basis to ensure accurate design of the mixing tank [21].

B. Mathematical modeling of the mixing tank

A mathematical model was developed for the mixing tank shown in Fig. 1. Streams F_1, F_2, F_3, and F_4 correspond to the feed flow rates of solutions 1, 2, 3, and 4 in Table 2, respectively, whereas stream F_5 corresponds to the product flow rate. The mixing of the four feed streams was carried out in a stirred tank, with the outlet stream located at the bottom of the tank. The liquid volume within the tank was considered as the system for modeling purposes. On the other hand, the liquid level in the tank (h) was taken into account due to its importance in the operation and control of both mixing tanks and other chemical processes [22], [23], [24].

TABLE 2. CHEMICAL COMPOSITION OF THE FEED AND PRODUCT STREAMS IN THE MIXING TANK (MASS BASIS).

Component	**Solution 1**	**Solution 2**	**Solution 3**	**Solution 4**	**Solution 5**
	Mass fraction	***Mass fraction***	***Mass fraction***	***Mass fraction***	***Mass fraction***
Ethanol	0.9501	0	0	0	0.7565
Water	0.0499	0.9572	0.0159	1	0.2196
Glycerol	0	0	0.9841	0	0.0218
Hydrogen peroxide	0	0.0428	0	0	0.0021

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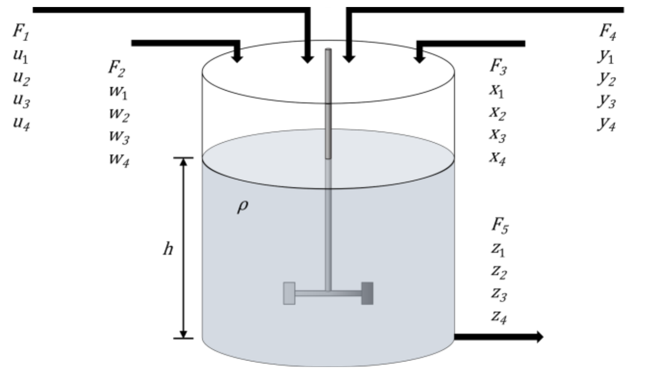

Fig. 1. Process flow diagram of the mixing tank, showing the process variables associated with the equations of the mathematical model employed in the design stage for handrub production.

Table 3 presents the dynamic mathematical model for the system studied. The model equations were derived from the law of conservation of matter, assuming perfect mixing, isothermal operation, and constant system density. The tank volume was defined in terms of the liquid level height and the tank cross-sectional area. Accordingly, the mass flow rate of the outlet stream was expressed as a function of the liquid level of the tank, density, and a constant that depends on the valve flow coefficient [25].

TABLE 3. DYNAMIC MATHEMATICAL MODEL OF THE MIXING TANK FOR HANDRUB PRODUCTION.

Equation	Description
$\rho A \frac{dh}{dt} = F_1 + F_2 + F_3 + F_4 - F_5$	Total mass balance
$\rho A \frac{dz_1 h}{dt} = u_1 F_1 + w_1 F_2 + x_1 F_3 + y_1 F_4 - z_1 F_5$	Mass balance of ethanol
$\rho A \frac{dz_2 h}{dt} = u_2 F_1 + w_2 F_2 + x_2 F_3 + y_2 F_4 - z_2 F_5$	Mass balance of water
$\rho A \frac{dz_3 h}{dt} = u_3 F_1 + w_3 F_2 + x_3 F_3 + y_3 F_4 - z_3 F_5$	Mass balance of glycerol
$u_1 + u_2 + u_3 + u_4 = 1$	Summation constraints
$w_1 + w_2 + w_3 + w_4 = 1$	Summation constraints
$x_1 + x_2 + x_3 + x_4 = 1$	Summation constraints
$y_1 + y_2 + y_3 + y_4 = 1$	Summation constraints
$z_1 + z_2 + z_3 + z_4 = 1$	Summation constraints
$F_5 = K\rho\sqrt{h}$	Mass flow rate of the outlet stream as a function of the liquid level of the tank

Where:
h is the liquid level of the tank.
ρ is the density of the liquid in the tank.
K is a constant that depends on the valve flow coefficient.
F_1, F_2, F_3 y F_4 are the mass flow rates of the inlet streams.
F_5 is the mass flow rate of the outlet stream.
u_i, w_i, x_i, y y_i are the mass fraction of the inlet streams F_1, F_2, F_3 y F_4, respectively.
z_i is the mass fraction of the outlet stream F_5.
Let the subscript i = 1, 2, 3, 4 denote components ethanol, water, glycerol and hydrogen peroxide, respectively.

In addition, constraints such as the condition that the sum of the mass fractions of all streams equals unity were included as additional equations. Based on these considerations, a total of ten equations constitute the mathematical model for the mixing tank studied.

C. Conceptual design of the mixing system

A conceptual design of the mixing tank was carried out to determine the nominal process variables. A steady-state mathematical model was obtained by modifying the dynamic model in Table 1. Table 4 presents the steady-state model, prepared for simulation purposes, which consists of algebraic equations set to zero. As can be observed, the accumulation terms in the mass balances were set to zero.

An analysis of degrees of freedom was performed to define the solution strategy for the mathematical model. Table 5 presents the degrees of freedom analysis for the steady-state model. Two model parameters (ρ, K) were identified. The values of ρ and K were taken as 857.33 kg/m^3 and 0.3132 m^3/h·m$^{1/2}$, respectively. On the other hand, a total of 26 variables and 10 equations were quantified, resulting in 16 degrees of freedom to be estimated. The number of degrees of freedom corresponds to the number of design variables for the mixer.

TABLE 4. STEADY-STATE MODEL OF THE MIXING TANK FOR HANDRUB PRODUCTION.

Equation	Number of equations
$F_1 + F_2 + F_3 + F_4 - F_5 = 0$	1
$u_1 F_1 + w_1 F_2 + x_1 F_3 + y_1 F_4 - z_1 F_5 = 0$	2
$u_2 F_1 + w_2 F_2 + x_2 F_3 + y_2 F_4 - z_2 F_5 = 0$	3
$u_3 F_1 + w_3 F_2 + x_3 F_3 + y_3 F_4 - z_3 F_5 = 0$	4
$u_1 + u_2 + u_3 + u_4 - 1 = 0$	5
$w_1 + w_2 + w_3 + w_4 - 1 = 0$	6
$x_1 + x_2 + x_3 + x_4 - 1 = 0$	7
$y_1 + y_2 + y_3 + y_4 - 1 = 0$	8
$z_1 + z_2 + z_3 + z_4 - 1 = 0$	9
$F_5 - K\rho\sqrt{h} = 0$	10

TABLE 5. DEGREES OF FREEDOM ANALYSIS FOR THE MATHEMATICAL MODEL OF THE MIXIG TANK IN THE DESING STAGE.

Step	Specification
1. Parámetros	ρ, K
2. Número de variables, N_V	26
3. Número de ecuaciones, N_E	10
4. Número de grados de libertad, N_F	$N_F = N_V - N_E = 26 - 10 = 16$
5. Variables de diseño	$F_5, u_1, u_2, u_3, w_2, w_3, w_4, x_1, x_2, x_3, y_1, y_2, y_3, z_1, z_3, z_4$
6. Variables de estado	$F_1, F_2, F_3, F_4, u_4, w_4, x_1, y_4, z_2, h$

A proposal for the 16 design variables was established, including the mass flow rate of the outlet stream and specific mass fractions of the inlet and outlet streams.

Table 6 presents the values for the specified design variables. The mass flow rate of the outlet stream was determined based on a target handrub production rate of 100 kg/h. The mass fractions of the feed streams were taken from the compositions of the solutions used as raw materials in the mixing process (see Table 2). In contrast, the composition values of the outlet stream were specified according to the product quality requirements of the mixing system, as shown for solution 5 in Table 2.

The conceptual design was carried out by solving the steady-state mathematical model. Ten state variables were estimated, among which were the liquid level of the tank and the flow rates of the feed streams. Fig. 2 shows the conceptual design of the mixing tank, including the nominal values of all process variables.

The nominal values of the feed streams F_1, F_2, F_3 and F_4 were calculated as 79.62, 4.91, 2.22, and 13.25 kg/h, respectively. Under steady-state operation of the mixing tank, these feed streams correspond to a nominal handrub production rate of 100 kg/h. It is noteworthy that the ethanol solution feed exhibits a substantially higher flow rate (79.62 kg/h) compared with the hydrogen peroxide and glycerol solution feeds (4.91 and 2.22 kg/h, respectively). In addition, a significant water stream (13.35 kg/h) is required to ensure that the product stream reaches its nominal composition of 75.65% (w/w).

Moreover, a nominal liquid level of 0.48 m was determined to achieve the target handrub production rate. The mixing tank diameter and system volume were subsequently estimated.

TABLE 6. SPECIFICATIONS OF DESIGN VARIABLES FOR THE SOLUTION OF THE STEADY-STATE MODEL OF THE MIXING TANK.

Design variable	Value	Design variable	Value	Design variable	Value
F_5 (kg/h)	100	w_4	0.0428	y_3	0
u_1	0.9501	x_1	0	z_1	0.7565
u_2	0.0499	x_2	0.0159	z_3	0.0218
u_3	0	x_3	0.9841	z_4	0.0021
w_2	0.9572	y_1	0		
w_3	0	y_2	1		

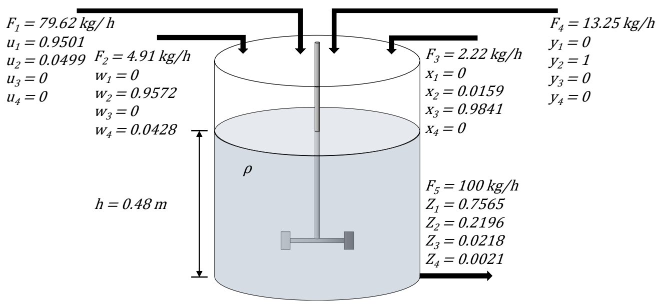

Fig. 2. Conceptual design of the mixing tank for handrub production.

For mixing operations in stirred tanks, a liquid height-to-diameter ratio between 0.8 and 2 is generally recommended [26], [27], [28]. Accordingly, a ratio of 1 was selected, resulting in a tank diameter of 0.48 m and a liquid volume of 0.087 m³. These results provide a basis for future studies on the operation and control of the mixing tank.

IV. CONCLUSIONS

A conceptual design of a mixing tank for alcohol-based handrub production was developed using a steady-state mathematical model. Nominal feed and product compositions were determined, demonstrating the predominance of the ethanol stream and the required water addition to achieve 75.65% (w/w) ethanol in the final product, according to the WHO quality specifications.

Sixteen design variables, including the outlet flow rate and selected mass fractions, were specified to ensure proper system operation. In addition, ten state variables, such as the liquid level and feed flow rates, were determined. A liquid level of 0.48 m and a tank diameter of 0.48 m (volume 0.087 m³) were established, providing a robust basis for future operation, control, and process optimization of the mixing system.

This study highlights the importance of mixing in the production of healthcare products, particularly alcohol-based hand sanitizers, whose design and operating policies are directly related to public health safety.

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