

Steady-State Availability Analysis of a Synthetic Ammonia Process Unit: A Mathematical Perspective

Zeenaat Zaidi

Department of Mathematics, College of Science, Qassim University, Buraidah 51452, Kingdom of Saudi Arabia

Email: z.hasain[at]qu.edu.sa

Abstract: *This study evaluates the steady-state availability of a synthetic ammonia process unit using a probabilistic mathematical framework based on the Markov birth-death process. First-order differential equations define system dynamics, and various failure and repair rates are analyzed to assess system performance. The results, presented through tabular and graphical representations, offer insights into potential system bottlenecks, aiding in reliability and maintenance optimization. By integrating advanced mathematical modeling with computational tools, this research provides a structured approach for enhancing efficiency and availability in ammonia manufacturing systems.*

Keywords: Steady-state availability, mathematical modeling, Markov process, reliability analysis, ammonia synthesis process

1. Introduction

Mathematics plays a crucial role in the chemical industry by aiding in the understanding, design, optimization, and control of various processes and systems. It is essential for enhancing efficiency, saving costs, and ensuring the safety and lifespan of chemical operations. Numerous researchers have examined the application of mathematics and mathematical modeling in the chemical industry. Applications of mathematical modeling in chemical engineering highlight the tool's versatility in addressing a wide range of problems, from process design to optimization, control, and environmental impact assessment. These models provide critical insights to engineers, helping them to make better-informed decisions, boost efficiency, and ensure the reliable and sustainable operation of chemical processes. The chemical industry is a varied and complicated sector with a significant impact on the global economy. It entails the manufacture, processing, and distribution of chemicals, which are substances with unique molecular compositions. Modak [1] explained the Haber process for the synthesis of ammonia. Ramkrishna and Amundson [2] examined the importance of mathematics in the field of chemical engineering. Elnashaie and Uhlig [3] created mathematical models for a variety of commercial operations by combining mass, momentum, and heat-balance equations with the rates of the processes that occur inside the system's boundaries. Models are solved numerically using MATLAB algorithms, with a focus on the design and optimization of chemical and biological industrial equipment and plants. Researchers have discussed the use of mathematical ideas and models to enhance a wide range of chemical processes, from reaction kinetics to boosting energy efficiency, controlling systems, and addressing environmental problems. Their coordinated efforts underscore the significance of mathematical modeling as a versatile tool that aids in well-informed choices and advances in the field of chemical engineering. Rasmuson et al. [4] developed, built, simplified, tested, and interpreted mathematical models in chemical engineering. Medford et al. [5] demonstrated a method for calculating the catalytic rate of ammonia synthesis over a spectrum of transition metal

catalysis. Luaces [6] investigated chemistry and biochemistry applications and modeling challenges.

The topic of availability has received a lot of attention in the literature. Calixto [7] confirmed the concept of system performance indices, which comprise production efficiency, availability, and reliability, and described how these performance indicators might be predicted. Ukpaka et al. [8] used the Haber process to investigate the reliability of functional parameters and coefficients on ammonia production in a fixed-bed reactor using hydrogen gas and nitrogen. Tian et al. [9] introduced a Markov chain-based error propagation model to analyze the reliability of component-based software systems and safeguard their critical components. Ren and Guo [10] proposed an approach for calculating dependability that uses a Markov chain-based error propagation model. Furthermore, Taj and Rizwan [11] did a thorough review of the literature on the modeling and analysis of the dependability of complex industrial systems. They assessed the many types of systems investigated, the variety of assumptions and operating settings considered, the research methodologies employed, and the ultimate conclusions of these investigations. Smith et al. [12] illustrated the current and future role of Haber-Bosch ammonia. Duan et al. [13] studied the ammonization of a Nafion membrane throughout tests, as well as the quantification underestimate. Finally, a reliable level of synthesized ammonia is discovered, and some recommendations are made to increase ammonia measurement reliability and accuracy. The synthetic ammonia process unit is a crucial ammonia production facility that is essential in many industrial sectors, notably fertilizer manufacturing. The Haber-Bosch process, often known as the synthetic ammonia process, is a technique for industrially producing ammonia (NH₃). Ammonia is a critical compound that is used in a variety of applications, most notably as a fertilizer in agriculture and as a building block for many chemical products. The process, developed in the early twentieth century by Fritz Haber and Carl Bosch, involves the reaction of nitrogen (N₂) from the air and hydrogen (H₂) from natural gas or other hydrocarbon sources

under high temperature and pressure in the presence of a catalyst to generate ammonia. Humphreys et al. [14] discussed recent advances in catalyst research, to provide an overview of the present state of catalysts utilized in ammonia synthesis.

Bahl and Garg [15] investigated the reliability of an ammonia plant in a transitory state and assessed it using a computer algebra system, Mathematica. Ghavam et al. [16] conducted a comprehensive study of numerous sustainable hydrogen generation techniques and developing technologies for sustainable ammonia synthesis, as well as a life cycle assessment of various ammonia production methods. Liu et al. [17] suggested a unique intelligent quantitative risk assessment approach (DYN - LSTM - QRA) for the ammonia synthesis process based on a dynamic mechanism model. Trivya et al. [18] investigated the safety, operability, and reliability of an ammonia fuel - cell - powered ship while taking bunkering and fuel specifications into account. Moustafa et al. [19] used Accelerated Life Testing (ALT) to provide a unique approach for testing the dependability of systems with multiple components. In a similar spirit, Jagtap et al. [20] conducted a detailed RAM (Reliability, Availability, and Maintainability) analysis to examine the performance of a water circulation system in a coal-fired power plant. Meanwhile, Maihulla et al. [21] investigated the reliability metrics of a three-system reverse osmosis filtration system. Spatolisano and Pellegrini [22] outlined the manufacturing of ammonia in smaller, dispersed facilities and investigated the intensification of the ammonia production process. They improved the procedure by adding an ammonia elimination stage by absorption using a phosphate solution. In a recent study, Khalilov [23] developed a comprehensive mathematical model for the Haber-Bosch process in ammonia synthesis, based on the foundational principles of mathematical physics.

This study investigates the steady-state availability of a synthetic ammonia process unit in depth. The study applies a careful analytical technique to assess the system's operational reliability and continuous functionality over a prolonged time. This research attempts to give a full knowledge of the unit's availability by concentrating on the probabilistic assessment of steady-state circumstances.

A complete evaluation of the synthetic ammonia process unit is investigated in this study to determine the long-run availability. Availability refers to the likelihood that the equipment will be available when it is needed. To increase productivity, the availability and dependability of operational systems/subsystems must be maintained at the greatest level. The most significant element is availability, which is directly connected to system productivity. As a result, system availability must be considered to achieve high output and high quality. To sustain system performance throughout the system's service life, it is vital to identify system constraints so that effective maintenance planning may be developed. The current study is useful in identifying system flaws and weak spots.

This examination focuses on determining the system's capacity to operate continuously without interruptions or outages, maintaining steady production. This research dives

into the intricate operational dynamics of the synthetic ammonia process unit using modern numerical approaches. Using probabilistic models, reliability analysis, and statistical techniques, the research attempts to quantify the system's availability under various operational scenarios, taking into account factors such as component reliability, failure rates, and maintenance tactics.

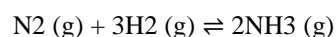
The underlying objective of this research is to provide a comprehensive knowledge of the steady-state availability of the synthetic ammonia process unit. This research attempts to give insights critical for enhancing the unit's operating efficiency and dependability by analyzing the reliability of individual components, failure mechanisms, maintenance methods, and related hazards. Long-term availability is also investigated using tables with varying repair rates. MATLAB 7.8.0 (R2009a) is used to create tables for steady-state availability. The findings are beneficial to chemical and reliability engineers.

The primary objective of this research is to evaluate the steady-state availability of a synthetic ammonia process unit using mathematical modeling. By examining failure and repair rates, this study aims to provide insights into optimizing system performance and reliability. This research is significant for chemical and reliability engineers as it provides a systematic approach to enhancing operational efficiency in ammonia production units. By identifying system constraints and optimizing failure-repair dynamics, it contributes to industrial process optimization.

2. Explanation of the System

2.1 The Haber-Bosch Method

An ammonia process unit in the chemical industry produces ammonia (NH₃) using a chemical synthesis process. Ammonia is an important chemical compound utilized in a variety of sectors, including agriculture, as a fertilizer, and in the manufacture of chemicals, and medicines. Nitrogen is derived from the atmosphere, which contains around 78% nitrogen. Natural gas, namely methane (CH₄), is used to produce hydrogen, while other hydrocarbons or water electrolysis can also be used. To ensure the effectiveness of the catalytic process, both nitrogen and hydrogen must be purified to remove contaminants.



The Haber-Bosch method was critical in revolutionizing agriculture by permitting large-scale manufacture of synthetic fertilizers. A combination of ammonia synthetic gas (with a ratio of 3 moles pure H₂ to 1 mole pure N₂) is compressed to an operational pressure ranging from 100 to 1000 atoms, depending on the required conversion. It is filtered to remove compression oil and then passed through a high temperature guard converter (CO and CO₂ to CH₄ and eliminates traces of H₂O, H₂S, P, and As). This is accomplished using a catalyst and appropriate getter materials. The comparatively cool gas is introduced along the exterior of the converter tube walls to provide cooling, permitting the use of carbon steel for the thick-walled pressure vessel and interval tubes. At temperatures ranging

from 500 to 550 degrees Celsius, the warmed gas travels through the inside of the tube, which houses a promoted porous iron catalyst. The resultant NH₃ product is extracted by condensation, initially through water cooling and then through NH₃ refrigeration, with approximately 8-30% conversion depending on process circumstances. The transformed N₂-H₂ mixture is recirculated to reach a yield of 85-90%. It can be stored or further processed for various applications. .

2.2 System Description

The synthetic ammonia process system consists of five subsystems namely Compressor, Oil Filter, Reactor, Water Chiller and Separator, two of them (Compressor and Separator) in reduced state.

- Compressor (A): Consists of two identical units which are subjected to minor and major failure.
- Oil Filter (B): Consists of one unit which is subjected to minor and major failure.
- Reactor (C): Consists of one unit which is subjected to minor and major failure.
- Water Chiller (D): Consists of one unit which is subjected to minor and major failure.
- Separator (E): Consists of two identical units which are subjected to minor and major failure.

2.3 Assumptions and Notations

The following are the basic assumptions used to develop the mathematical model:

- Failure and repair rates are statistically independent and stay stable throughout time.
- A repaired unit is deemed to be as capable as a new unit in terms of performance for a specified duration.
- There are several repair services accessible.
- Standby units are similar to active units in every way.
- Repair and/or replacement are both included in the service.
- The system is capable of operating at reduced capacity.

A, B, C, D, E: Subsystems in good operating state.

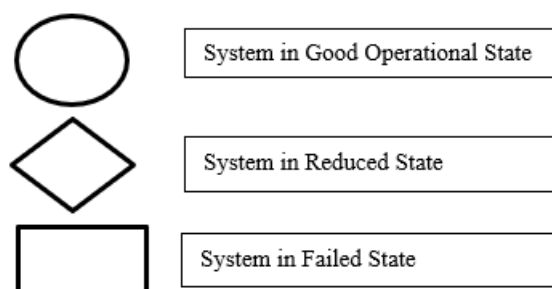
a, b, c, d, e: Indicates the failed state of A, B, C, D and E.

\bar{A} , \bar{E} : Indicates that the subsystems A and E are working at reduced capacity.

α_i ($i = 1, 2, 3, 4, 5, 6, 7$): Represents failure rates of the subsystems A, \bar{A} , B, C, D, E, \bar{E}

β_i ($i = 1, 2, 3, 4, 5, 6, 7$): Represents repair rates of the subsystems \bar{A} , a, b, c, d, \bar{E} and e

$P_i(t)$: Probability the system is in i^{th} state at time t .



2.4 Transition Diagram of the System

Based on these assumptions and notations, transition diagram is developed as shown in **Figure 1**.

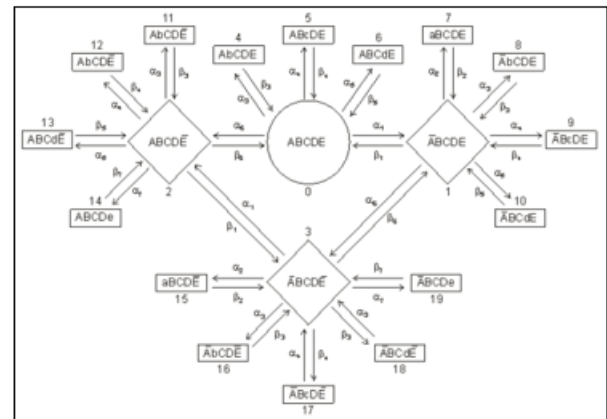


Figure 1: Transition Diagram

3. Mathematical Modeling of the Synthetic Ammonia Process Unit System

A Markov model describes the probability of different system states across time, allowing you to examine the time-dependent dependability of components. This strategy is useful when the failure and repair rates are consistent. The system's state behavior is driven by a Markov process, in which the probability of transitioning to future states is purely determined by the present state, regardless of the system's previous history. The variables that define this process are state and time.

The system of linear differential equations is developed by means of mnemonic rule. The differential equations can be written as,

$$P'_0(t) + (\alpha_1 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6)P_0(t) = \beta_1P_1(t) + \beta_3P_4(t) + \beta_4P_5(t) + \beta_5P_6(t) + \beta_6P_2(t)$$

$$P'_1(t) + (\alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \beta_1)P_1(t) = \beta_2P_7(t) + \beta_3P_8(t) + \beta_4P_9(t) + \beta_5P_{10}(t) + \beta_6P_3(t) + \alpha_1P_0(t)$$

$$P'_2(t) + (\alpha_1 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_7 + \beta_6)P_2(t) = \beta_3P_{11}(t) + \beta_4P_{12}(t) + \beta_5P_{13}(t) + \beta_7P_{14}(t) + \beta_1P_3(t) + \alpha_6P_0(t)$$

$$P'_3(t) + (\alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_7 + \beta_1 + \beta_6)P_3(t) = \beta_2P_{15}(t) + \beta_3P_{16}(t) + \beta_4P_{17}(t) + \beta_5P_{18}(t) + \beta_7P_{19}(t) + \alpha_1P_2(t) + \alpha_6P_1(t)$$

$$P'_4(t) + \beta_3P_4(t) = \alpha_3P_0(t)$$

$$P'_5(t) + \beta_4P_5(t) = \alpha_4P_0(t)$$

$$P'_6(t) + \beta_5P_6(t) = \alpha_5P_0(t)$$

$$P'_7(t) + \beta_2P_7(t) = \alpha_2P_1(t)$$

$$P'_8(t) + \beta_3P_8(t) = \alpha_3P_1(t)$$

$$P'_9(t) + \beta_4P_9(t) = \alpha_4P_1(t)$$

$$P'_{10}(t) + \beta_5P_{10}(t) = \alpha_5P_1(t)$$

$$P'_{11}(t) + \beta_3P_{11}(t) = \alpha_3P_2(t)$$

$$P'_{12}(t) + \beta_4P_{12}(t) = \alpha_4P_2(t)$$

$$P'_{13}(t) + \beta_5 P_{13}(t) = \alpha_5 P_2(t)$$

$$P'_{14}(t) + \beta_7 P_{14}(t) = \alpha_7 P_2(t)$$

$$P'_{15}(t) + \beta_2 P_{15}(t) = \alpha_2 P_3(t)$$

$$P'_{16}(t) + \beta_3 P_{16}(t) = \alpha_3 P_3(t)$$

$$P'_{17}(t) + \beta_4 P_{17}(t) = \alpha_4 P_3(t)$$

$$P'_{18}(t) + \beta_5 P_{18}(t) = \alpha_5 P_3(t)$$

$$P'_{19}(t) + \beta_7 P_{19}(t) = \alpha_7 P_3(t)$$

With initial conditions at time $t = 0$,

$$P_i(t) = 1 \text{ for } i = 0 \\ = 0 \text{ for } i \neq 0$$

Steady-state Availability

The management is always interested in long run availability of the system. Long run availability may be calculated by considering the fact that $\frac{d}{dt} \rightarrow 0$ as $t \rightarrow \infty$. The differential difference equations reduce to:

$$(\alpha_1 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6)P_0 = \beta_1 P_1 + \beta_3 P_4 + \beta_4 P_5 + \beta_5 P_6 + \beta_6 P_2$$

$$(\alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \beta_1)P_1 \\ = \beta_2 P_7 + \beta_3 P_8 + \beta_4 P_9 + \beta_5 P_{10} \\ + \beta_6 P_3 + \alpha_1 P_0$$

$$(\alpha_1 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_7 + \beta_6)P_2 \\ = \beta_3 P_{11} + \beta_4 P_{12} + \beta_5 P_{13} + \beta_7 P_{14} \\ + \beta_1 P_3 + \alpha_6 P_0$$

$$(\alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_7 + \beta_1 + \beta_6)P_3 \\ = \beta_2 P_{15} + \beta_3 P_{16} + \beta_4 P_{17} + \beta_5 P_{18} \\ + \beta_7 P_{19} + \alpha_1 P_2 + \alpha_6 P_1$$

$$\beta_3 P_4 = \alpha_3 P_0$$

$$\beta_4 P_5 = \alpha_4 P_0$$

$$\beta_5 P_6 = \alpha_5 P_0$$

$$\beta_2 P_7 = \alpha_2 P_1$$

$$\beta_3 P_8 = \alpha_3 P_1$$

$$\beta_4 P_9 = \alpha_4 P_1$$

$$\beta_5 P_{10} = \alpha_5 P_1$$

$$\beta_3 P_{11} = \alpha_3 P_2$$

$$\beta_4 P_{12} = \alpha_4 P_2$$

$$\beta_5 P_{13} = \alpha_5 P_2$$

$$\beta_7 P_{14} = \alpha_7 P_2$$

$$\beta_2 P_{15} = \alpha_2 P_3$$

$$\beta_3 P_{16} = \alpha_3 P_3$$

$$\beta_4 P_{17} = \alpha_4 P_3$$

$$\beta_5 P_{18} = \alpha_5 P_3$$

$$\beta_7 P_{19} = \alpha_7 P_3$$

Solving above equations, we get

$$(\alpha_1 + \alpha_6)P_0 = \beta_1 P_1 + \beta_6 P_2$$

$$(\alpha_6 + \beta_1)P_1 = \beta_6 P_3 + \alpha_1 P_0$$

$$(\alpha_1 + \beta_6)P_2 = \beta_1 P_3 + \alpha_6 P_0$$

$$(\beta_1 + \beta_6)P_3 = \alpha_1 P_2 + \alpha_6 P_1$$

After solving these equations recursively, we get all the probabilities in terms of P_0

$$P_1 = \frac{\alpha_1}{\beta_1} P_0$$

$$P_2 = \frac{\alpha_6}{\beta_6} P_0$$

$$P_3 = \frac{\alpha_1 \alpha_6}{\beta_1 \beta_6} P_0$$

Using the normalizing condition, we obtain $P_0, \sum_{i=0}^{19} P_i = 1$

$$P_0 = \left[1 + \frac{\alpha_1}{\beta_1} + \frac{\alpha_6}{\beta_6} + \frac{\alpha_1 \alpha_6}{\beta_1 \beta_6} + \frac{\alpha_3}{\beta_3} + \frac{\alpha_4}{\beta_4} \right. \\ + \frac{\alpha_5}{\beta_5} + \frac{\alpha_1 \alpha_2}{\beta_1 \beta_2} + \frac{\alpha_1 \alpha_3}{\beta_1 \beta_3} + \frac{\alpha_1 \alpha_4}{\beta_1 \beta_4} + \frac{\alpha_1 \alpha_5}{\beta_1 \beta_5} \\ + \frac{\alpha_3 \alpha_6}{\beta_3 \beta_6} + \frac{\alpha_4 \alpha_6}{\beta_4 \beta_6} + \frac{\alpha_5 \alpha_6}{\beta_5 \beta_6} + \frac{\alpha_6 \alpha_7}{\beta_6 \beta_7} + \frac{\alpha_1 \alpha_2 \alpha_6}{\beta_1 \beta_2 \beta_6} \\ \left. + \frac{\alpha_1 \alpha_3 \alpha_6}{\beta_1 \beta_3 \beta_6} + \frac{\alpha_1 \alpha_4 \alpha_6}{\beta_1 \beta_4 \beta_6} + \frac{\alpha_1 \alpha_5 \alpha_6}{\beta_1 \beta_5 \beta_6} + \frac{\alpha_1 \alpha_6 \alpha_7}{\beta_1 \beta_6 \beta_7} \right]^{-1}$$

The steady state availability of the system is given by

$$\text{Availability} = P_0 + P_1 + P_2 + P_3 \\ = \left(1 + \frac{\alpha_1}{\beta_1} + \frac{\alpha_6}{\beta_6} + \frac{\alpha_1 \alpha_6}{\beta_1 \beta_6} \right) P_0$$

4. Steady-State Analysis

The limiting probabilities from the aforementioned equations were calculated using a recursive technique and a normalizing condition with time t tending to infinity for steady-state availability evaluation. The performance matrices, which are given in Table 1 through Table 4, were created using MATLAB 7.8.0 (R2009a). These matrices depict various degrees of availability for various combinations of failure and repair rates. The Availability of the system was assessed by evaluating different combinations of failure and repair rates within its subsystems. Through statistical analysis, this strategy is intended to improve understanding of the system's performance. Figure 2 to Figure 5 demonstrates the system's availability as a function of various failure and repair rates. These graphs, prepared in Microsoft Excel, give a more thorough understanding of how different failure and repair rates within each subsystem affect system availability.

4.1 Impact of Failure Rate (α_1) and Repair Rate (β_1) of Compressor on Long-run Availability.

Failure and Repair rates of compressor are taken as

$$\alpha_1 = 0.001, \quad 0.002, \quad 0.003, \quad 0.004$$

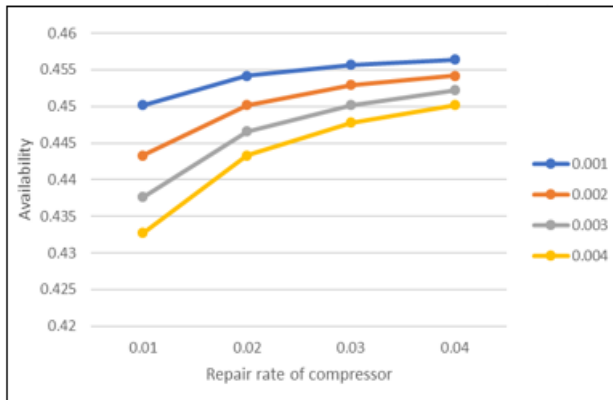
$$\beta_1 = 0.01, \quad 0.02, \quad 0.03, \quad 0.04$$

Other failure and repair rates of the subsystems have been taken as: $\alpha_2 = 0.002, \alpha_3 = 0.002, \alpha_4 = 0.0015, \alpha_5 = 0.001, \alpha_6 = 0.001, \alpha_7 = 0.0025, \beta_2 = 0.012, \beta_3 = 0.015, \beta_4 = 0.1, \beta_5 = 0.001, \beta_6 = 0.01, \beta_7 = 0.002$.

Using these values, long-run availability of the system is calculated and has been tabulated in **Table 1**.

Table 1: Impact of Failure and Repair Rate of Compressor on Long-run Availability

α_1/β_1	0.01	0.02	0.03	0.04
0.001	0.4502	0.4542	0.4557	0.4564
0.002	0.4433	0.4502	0.4529	0.4542
0.003	0.4376	0.4466	0.4502	0.4522
0.004	0.4327	0.4433	0.4478	0.4502

**Figure 2:** Impact of Failure and Repair Rate of Compressor on Long-run Availability

An increase in repair rates from 0.01 to 0.04 resulted in a noticeable rise in availability, reaching 1.37% to 4%. Conversely, an escalation in failure rates from 0.001 to 0.004 led to a decrease in availability by 3.88%.

4.2 Impact of Failure Rate (α_3) and Repair Rate (β_3) of Oil Filter on Long-run Availability.

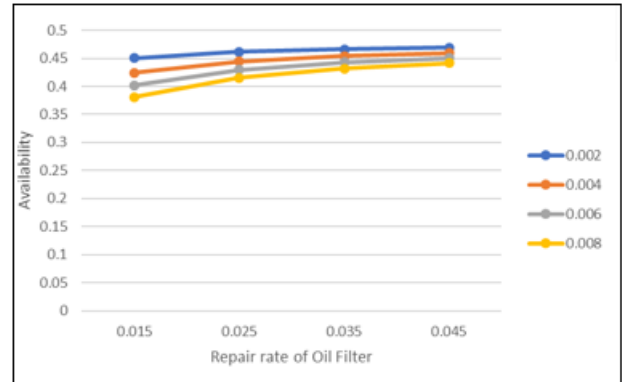
Failure and Repair rates of Oil Filter are taken as
 $\alpha_3 = 0.002, 0.004, 0.006, 0.008$
 $\beta_3 = 0.015, 0.025, 0.035, 0.045$

Other failure and repair rates of the subsystems have been taken as: $\alpha_1 = 0.001, \alpha_2 = 0.002, \alpha_4 = 0.0015, \alpha_5 = 0.001, \alpha_6 = 0.001, \alpha_7 = 0.0025,$
 $\beta_1 = 0.01, \beta_2 = 0.012, \beta_4 = 0.1, \beta_5 = 0.001, \beta_6 = 0.01, \beta_7 = 0.002.$

Using these values, long-run availability of the system is calculated and has been tabulated in **Table 2**.

Table 2: Impact of Failure and Repair Rate of Oil Filter on Long-run Availability.

α_3/β_3	0.015	0.025	0.035	0.045
0.002	0.4502	0.4614	0.4664	0.4692
0.004	0.4245	0.4448	0.4542	0.4595
0.006	0.4016	0.4294	0.4426	0.4502
0.008	0.3810	0.4151	0.4316	0.4413

**Figure 3:** Impact of Failure and Repair Rate of Oil Filter on Long-run Availability.

Increasing repair rates from 0.015 to 0.045 resulted in a substantial availability increase of 4.22% to 15.82%. However, a rise in failure rates from 0.002 to 0.008 caused a notable availability decrease of 15.37%.

4.3 Impact of Failure Rate (α_4) and Repair Rate (β_4) of Reactor on Long-run Availability.

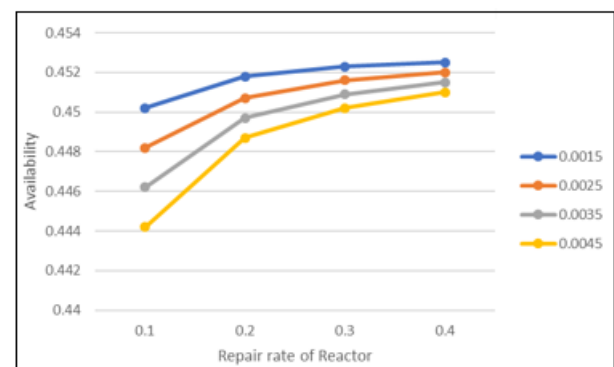
Failure and Repair rates of Reactor are taken as
 $\alpha_4 = 0.001, 0.002, 0.003, 0.004$
 $\beta_4 = 0.1, 0.02, 0.03, 0.04$

Other failure and repair rates of the subsystems have been taken as: $\alpha_1 = 0.001, \alpha_2 = 0.002, \alpha_3 = 0.002, \alpha_5 = 0.001, \alpha_6 = 0.001, \alpha_7 = 0.0025,$
 $\beta_1 = 0.01, \beta_2 = 0.012, \beta_3 = 0.015, \beta_5 = 0.001, \beta_6 = 0.01, \beta_7 = 0.002.$

Using these values, long-run availability of the system is calculated and has been tabulated in **Table 3**.

Table 3: Impact of Failure and Repair Rate of Reactor on Long-run Availability

α_4/β_4	0.1	0.2	0.3	0.4
0.0015	0.4502	0.4518	0.4523	0.4525
0.0025	0.4482	0.4507	0.4516	0.4520
0.0035	0.4462	0.4497	0.4509	0.4515
0.0045	0.4442	0.4487	0.4502	0.4510

**Figure 4:** Impact of Failure and Repair Rate of Reactor on Long-run Availability

Elevating repair rates from 0.1 to 0.4 led to an availability increase of 0.51% to 1.53%. Conversely, an increase in failure rates from 0.0015 to 0.0045 resulted in a decreased availability of 1.33%.

4.4 Impact of Failure Rate (α_5) and Repair Rate (β_5) of Waterchiller on Long-run Availability.

Failure and Repair rates Waterchiller are taken as

$$\alpha_5 = 0.001, \quad 0.002, \quad 0.003, \quad 0.004$$

$$\beta_5 = 0.001, \quad 0.0015, \quad 0.002, \quad 0.0025$$

Other failure and repair rates of the subsystems have been taken as: $\alpha_1 = 0.001$, $\alpha_2 = 0.002$, $\alpha_3 = 0.002$, $\alpha_4 = 0.015$, $\alpha_6 = 0.001$, $\alpha_7 = 0.0025$, $\beta_1 = 0.01$, $\beta_2 = 0.012$, $\beta_3 = 0.015$, $\beta_4 = 0.1$, $\beta_6 = 0.01$, $\beta_7 = 0.002$.

Using these values, long-run availability of the system is calculated and has been tabulated in **Table 4**.

Table 4: Impact of Failure and Repair Rate of Waterchiller on Long-run Availability.

α_5/β_5	0.001	0.002	0.003	0.004
0.001	0.4502	0.5686	0.6233	0.6547
0.0015	0.3721	0.5015	0.5673	0.6071
0.002	0.3170	0.4485	0.5205	0.5660
0.0025	0.2762	0.4057	0.4809	0.5300

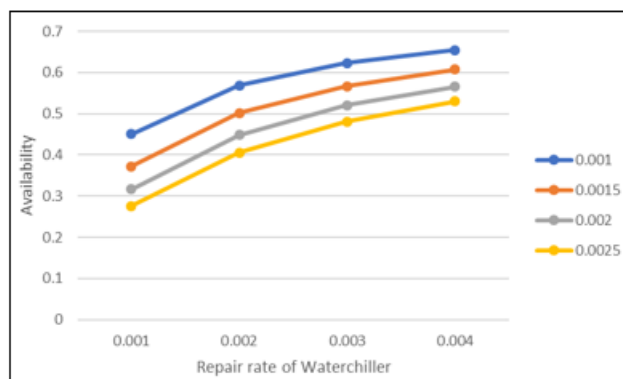


Figure 5: Impact of Failure and Repair Rate of Waterchiller on Long-run Availability

A significant rise in availability occurred when repair rates were increased from 0.001 to 0.004, reaching 45.42% to 91.89%. However, an increase in failure rates from 0.001 to 0.0025 caused a substantial availability decrease of 38.64%.

5. Conclusion

A comparative analysis of the tables indicates that the Water Chiller subsystem (D) has the most pronounced influence on the overall system performance. The Oil Filter subsystem (B) also exerts a modest impact on system availability. Conversely, the Compressor, Reactor, and Separator subsystems exhibit relatively uniform effects on system performance. Consequently, it is advisable for management and chemical engineers to prioritize attention to subsystems B and D in order to enhance overall system availability. Across all subsystems (A, B, C, and D), heightened repair rates consistently demonstrated a positive correlation with increased availability. Conversely, increased failure rates consistently resulted in decreased availability for all subsystems, emphasizing a negative correlation between failure rate and availability.

Optimizing repair rates proves to be a pivotal factor in enhancing the availability of subsystems within the synthetic ammonia process unit. However, the criticality of managing and controlling failure rates is underscored by their substantial impact on availability. Implementing strategies to minimize failure rates while maximizing repair rates could significantly improve the overall operational reliability and sustainability of the synthetic ammonia process unit. These findings underscore the importance of optimizing repair rates and minimizing failures to enhance operational efficiency. Future research should explore real-time predictive maintenance strategies to further improve system availability in industrial ammonia synthesis.

6. Discussion

Mathematics plays a crucial role in chemical research, manufacturing, and process optimization. Here are a few examples of how mathematics is used in the chemical industry:

- **Reaction Engineering and Chemical Kinetics:** To characterize the speeds of chemical processes and the mechanisms involved, differential equations and mathematical models are utilized. Reaction engineering concepts aid in the optimization of reaction conditions and the construction of reactors for efficient manufacturing processes.
- **Mass and Energy Balances:** In chemical processes, mathematical modeling is used to assure mass and energy conservation. Material and energy balances are critical for chemical process design and operation.
- **Process Optimization:** Mathematical optimization techniques are used to improve different processes, such as reactions, temperature, pressure, and flow rates, to maximize the result while minimizing energy consumption.
- **Statistical Process Control (SPC):** Statistical approaches are utilized in chemical process quality control and monitoring. Control charts and statistical analysis are tools that assist in discovering and managing differences in output.
- **Thermodynamic equations:** Thermodynamic equations are used to clarify and forecast the behavior of chemical reactions under different scenarios. Heat transfer equations aid in the design and optimization of heat exchangers and other types of equipment.
- **Analytical Chemistry:** Analytical chemistry is the application of mathematical tools to evaluate and analyze experimental data collected from analytical equipment. Statistical evaluation, and mathematical representation all help with reliable chemical property measurement and analysis.
- **Computational Fluid Dynamics (CFD):** In numerous chemical processes, mathematical models and numerical illustrations are used to investigate fluid flow, heat transport, and mass transfer. CFD aids in the optimization of equipment design and the enhancement of overall process efficiency.
- **Environmental Impact Assessment:** To analyze and anticipate the ecological effects of chemical processes, mathematical modeling is applied. This involves modeling pollution dispersal, monitoring air and water quality, and forecasting the impact on ecosystems.

- Supply Chain Optimization: Mathematical models optimize supply chains by managing inventory, logistics, and production scheduling.
- Materials Science: Mathematical representations are used in materials science to predict material qualities such as durability, flexibility, and heat transfer. Computational approaches aid in the development of novel materials for certain uses.

References

- [1] J. M. Modak, Haber Process for Ammonia Synthesis, *Resonance* 7(9) (2002) 69-77.
- [2] D. Ramkrishna, N. R. Amundson, Mathematics in chemical engineering: A 50-year introspection. *AIChE Journal*, 50 (2004) 7-23.
- [3] S. S. E. H. Elnashaie, F. Uhlig, Numerical Techniques for Chemical and Biological Engineers using MATLAB ® A Simple Bifurcation Approach, Springer, 2007.
- [4] A. Rasmuson, B. Anderson, L. Olsson, R. Anderson, Mathematical Modeling in Chemical Engineering, Cambridge University Press, 2014.
- [5] A. J. Medford, A. Vojvodic, F. Studt, J. Wellendorff, Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates, *Science* 345 (2014) 197-200.
- [6] V. M. Luaces, Mathematical models for chemistry and biochemistry service courses, CERME 9 - Ninth Congress of the European Society for Research in Mathematics Education, Charles University in Prague, Faculty of Education, ERME, Prague, Czech Republic, (2015) 904-909.
- [7] E. Calixto, Reliability, Availability, and Maintainability (RAM) Analysis. Book: Gas and Oil Reliability Engineering, second edition, 269-470, 2016.
- [8] C. P. Ukpaka, T. Izonowei, Model prediction on the reliability of fixed bed reaction for ammonia production. *Chemistry International*, 3(1) (2017) 46-57.
- [9] Z. Tian, Y. Wang, P. Zong, A Markov error propagation model for component-based software systems. *International Journal of Performability Engineering* 14(9) (2018) 2030-2039.
- [10] W. Ren, B. Guo, Research on Reliability analysis of Component-based software. *Advances in Engineering Research*, 139 (2018) 226-232.
- [11] S. Z. Taj, S. M. Rizwan, Reliability modelling and analysis of complex industrial systems - A Review, *I-Manager's Journal on Mathematics*, 8(2) (2019) 43-60.
- [12] C. Smith, A. K. Hill, L. T. Murciano, Current and Future role of Haber-Bosch ammonia in a carbon-free energy landscape, *Energy & Environmental Science* 13 (2020) 331-344.
- [13] G. Y. Duan, Y. Ren, Y. Tang, Y. Z. Sun, Y. M. Chen, P. Y. Wan, X. J. Yang, Improving the Reliability and Accuracy of Ammonia Quantification in Electro and Photochemical Synthesis. *ChemSusChem*, 13(1) (2020) 88-96.
- [14] J. Humphreys, R. Lan, S. Tao, Development and Recent Progress on Ammonia Synthesis Catalysts for Haber-Bosch process, *Advanced Energy and Sustainability Research*, 2 (2020) 1-23.
- [15] Y. Bahl, T. K. Garg, Modified Modelling and Reliability measure of ammonia synthesis unit in a Fertilizer Plant. *Turkish Journal of Computer and Mathematics Education*, 12(10) (2021) 2189-2196.
- [16] S. Ghavam, M. Vahdati, I. A. G. Wilson, P. Styring, Sustainable Ammonia production processes, *Frontiers in Energy Research*, 9 (2021) Article 580808.
- [17] Z. Liu, W. Tian, Z. Cui, H. Wei, C. Li, An intelligent quantitative risk assessment method for ammonia synthesis process. *Chemical Engineering Journal*, 420(11) (2021) 129893.
- [18] N. L. Trivyza, M. Cheliotis, E. Boulougouris, G. Theotokatos, Safety and Reliability Analysis of an Ammonia-Powered Fuel-cell System. *Safety* 2021, 7(4) (2021) 80.
- [19] K. Moustafa, Z. Hu, Z. P. Mourelatos, I. Baseski, M. Majcher, System reliability analysis using component-level and system-level accelerated life testing, *Reliability Engineering and System Safety*, 214 (2021) 107755.
- [20] H. P. Jagtap, A. K. Bewoor, R. Kumar, M. H. Ahmadi, M. E. H. Assad, M. Sharifpur, RAM analysis and availability optimization of thermal power plant water circulation system using PSO. *Energy Reports*, 7 (2021) 1133-1153.
- [21] A. S. Maihulla, I. Yusuf, Reliability analysis of reverse osmosis Filtration System using COPULA. *Qualilty and Reliability Engineering*, 17 (2022) 163-177.
- [22] E. Spatolisano, L. A. Pellegrini, Haber-Bosch process intensification: A first step towards small-scale distributed ammonia production, *Chemical Engineering Research and Design*, 195 (2023), 651-661.
- [23] A. J. Khalilov, Mathematical modelling of Haber-Bosch process in ammonia synthesis based on mathematical physics equations, *International Journal of Advanced Technology and Natural Sciences*, vol. 1 (2024).