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# SAFETY, HEALTH, ENVIRONMENTAL AND ECONOMIC (SHEE) ASSESSMENT OF FERTILIZER PRODUCTION

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## Abstract

Safety, health, environmental and economic (SHEE) assessment of a chemical process can be done either during process design stage or on existing plant. Although SHEE assessment during process design stage is more challenging due to the limited data availability, early assessment is advantageous as it provides more freedom for engineers to make process modification at lower cost rather than at later stages. Besides, considering SHEE earlier when developing a new plant may result in a more cost efficient, more controllable as well as environmentally friendlier and inherently safer and healthier process. This paper presents SHEE assessment for fertilizer production based on chemical routes. The safety, health and environmental assessment using Inherent Benign-ness Index (IBI) and Inherent Chemical Process Properties Data is demonstrated using ammonium nitrate and ammonium sulphate production as the case study. Both methods agree with each other that the chemical route for ammonium nitrate is inherently more benign than the ammonium sulphate production. The economic assessment based on gross profit analysis reveals that ammonium nitrate production is more profitable compared to the production of ammonium sulphate. This framework enables economic and SHE comparison for different chemical routes to help identify the most sustainable process at cost competitive.

***Keywords:*** SHE Assessment, Chemical Process Route, Fertilizer Production, Inherent Benign-ness Index (IBI), Inherent Chemical Process Properties Data

## 1.0 INTRODUCTION

The advanced technologies and economic achievements in modern development brought by chemical industries are one of the main factors that help in upgrading human lifestyle and economic health throughout the nations by offering important products ranging from health care to food processing [1]. Civilians have negative image towards chemical process industry. Somehow the process industry itself is to be blame due to activities that may contribute to serious environmental problems, climate changes and exposing workers and public to safety and health risk if not properly controlled. Currently, most SHE assessment methods compare process routes according to safety, health and environmental only. Qualitative and quantitative assessments of SHE performance of a chemical plant can be conducted at various stages of process design. Various methods have been introduced to assist engineers in designing sustainable plant notably the Dow Fire and Explosion Index (F&EI) [2] for safety and Life Cycle Analysis [3] for environment. The assessment presented by this paper will also include economic aspect in order to compare the process routes on term of cost competitive.

Safety, health, environmental and economic (SHEE) assessment of chemical processes can be done either on an existing plant or during process design stage. One advantage of the former one is the abundant data availability compared to during process design. However, early consideration of sustainability aspect during the development of a new plant or even for plant expansion, may result in a more cost efficient, more controllable as well as environmentally friendlier and inherently safer and healthier process. This study aims to evaluate the SHEE of two chemical routes in fertilizer production which are ammonium nitrate and ammonium sulphate by using two methods of Inherent Benign-ness Index (IBI) [4] and Inherent Chemical Process Properties Data [5] for safety, health and environmental aspects and using gross profit analysis for economic aspect.

## 2.0 EXISTING SHE ASSESSMENT METHODS FOR PROCESS DESIGN STAGE

Several methods have been introduced for sustainability assessment during process design stage for example the Integrated Inherent Safety Index (I2SI) [10], SHE method [11], IDEF0 method

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[12], INSET Toolkit [14], Inherent Benign-ness Index (IBI) [4] and Inherent Chemical Process Properties Data [5].

Integrated Inherent Safety Index (I2SI) integrates safety assessment with cost evaluation [10]. This index consists of two sub-indices which are Hazard Index (HI) and Inherent Safety Potential Index (ISPI). The damage possibility of a process with process and hazard control measures are evaluated by Hazard Index while Inherent Safety Potential Index considers the applicability of the inherent safety principles to the process.

A tool called SHE method presented by Koller *et al*., [11] provides solution to major limitation of sustainability assessment during process design stage as there are lack of input data for assessment during process design stage.

A method on management phase regarding evaluating safety, health and environmental assessments of plants during plant design stage was suggested by Sugiyama *et al.* [12]. This method is suitable for managers or project leaders to incorporate non-conventional environmental, health and safety evaluation of a design alternative. Type-zero method of Integrated DEFinition language or also known as IDEF0 is use in the evaluation. A design model comprises four design stages of process modeling and assessment that considers monetary and nonmonetary aspects is presented by Sugiyama *et al.* [3]. The four design stages include Process Chemistry I, Process Chemistry II, Conceptual Design I and Conceptual Design II. Reaction routes and process technologies alternatives are designed and assessed with the most promising options survive to the next stage. Indicators for evaluation at each stage covers economic performance, life-cycle environmental impacts and EHS hazard.

A method proposed by Carvalho *et al.,* focuses on the selection of the best alternatives of any chemical process [13]. Using SustainPro as the software, this method is able to prevent the typical trade off between competing design decisions.

The INSET Toolkit developed by The INSIDE Project Team Partners serves two functions [14]. The first function is as a means to raise the awareness of person involved in the process selection of a plant. Next, it function as a practical toolkit to be used by these persons as an integral part of the development, design and decision-making processes. This method covers four main stages which are chemical route selection, chemistry route detailed evaluation, process design optimization and process plant design. This toolkit use integration of safety, health and environmental hazards to ensure the effective management of the conflicts and synergies between these aspects.

Besides, another method that can be used is the Inherent Benign-ness Index (IBI) [4]. The IBI is a sustainability assessment method that integrates three sustainability criteria of safety, health and environmental in the assessment. This method focuses on assessment during design stage in order to choose the best chemical route among a selection of alternative chemical routes. This method is chosen to be used in our case study. Less benign route is represented by larger index number. However, this method has its own drawbacks although it does assess multi criteria. Detection of the most important factors for risk management is not considered since this method only considers basic information of the route such as reaction data and material properties [4]. A review of this method was done by Banimostafa *et al*. [15] for the potential application during process design stage.

Another alternative in conducting chemical route selection method is by applying multi-criteria decision making tool called the Inherent Chemical Process Properties Data [5]. This tool is used in choosing the optimized safety, health and environmental benigness level of a route. This method evaluates safety, health and environmental problems through the use of Inherent Safety Index (ISI) for safety assessment, Inherent Occupational Health Index (IOHI) is used as the reference in assessing health hazard while Environmental Hazard Index is used to assess environmental factor. Multi-criteria decision making is done by using Simple Additive Weighting (SAW) method which low total score indicates the most optimum safety, health and environmental characteristics. The application of this method is flexible as this method also

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enable user to choose a benign route either by individual assessments or integration of all three factors assessments. Users are able to determine their own preference regarding the priority of assessment in their plant for example prioritizing safety while the other two factors, health and environmental are treated with equal importance.

In this study, two methods are chosen in assessing the sustainability of ammonium nitrate and ammonium sulphate chemical routes which are the Inherent Benign-ness Index (IBI) and Inherent Chemical Process Properties Data.

## 3.0 METHODOLOGY

### 3.1 SHE Assessment Using Inherent Benign-ness Index (IBI)

The first step in Inherent Benign-ness Index (IBI) assessment is to assign the score values for every chemical in each parameter according to data provided by Material Safety Data Sheet (MSDS) while waste Reduction Algorithm Graphical User Interface (WAR GUI) software is used in obtaining the value for health and environmental parameters. The values are then normalized according to the equation provided by Srinivasan and Nahn [4] as tabulated in Table 1. Normalization is used as a scaling mean as each parameter does not share the same unit. Normalization is important so that all values evaluated can be added together for a final value representing a process route. All values were scaled so that they are in a range of between 0 and 1. As an example, the explosiveness parameter which involves values in the range of 0% to 100% of explosiveness limits is scaled to values in the range of 0 to 1 by dividing the explosiveness limits to 100. The normalized values will be added together into a Cumulative Index (CI) as shown in Eq (1). The larger the index value , represents less benign process route.

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**Table 1:** Factors Considered and their Normalization in Inherent Benign-ness Index (IBI) [4]

| Parameter | Typical Value | Original Range | Normalization Method |
|---|---|---|---|
| Toxicity (T) | [0,4] | [0,4] | $TOX_N = \frac{T}{4}$ |
| Reactivity (R) | [0,4] | [0,4] | $R_N = \frac{R}{4}$ |
| Explosiveness, E (%) | [0,100] | [0,100] | $E_N = \frac{E}{100}$ |
| Flammability (F) | [0,4] | [0,4] | $F_N = \frac{F}{4}$ |
| Heat of Reaction $\Delta H_R$ (kJ/mol) | [-600.600] | (-∞,+∞) | $\Delta H_{RN} = 1 - \frac{1}{1+a\times\Delta H_R^b}$<br>a= 4.47E-05<br>b= 2 |
| Pressure, P (atm) | [1,60] | (0,+∞) | P > 1 atm :<br>$P_N = 1\text{-}e^{-a(P-1)}$<br>a=0.03<br><br>P < 1 atm: |

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| | | | |
|---|---|---|---|
| | | | $P_N = 1-e^{a(P-1)}$<br>a=5 |
| Process Yield, Y (%) | [60,99] | [0,100] | $Y_N = \frac{100-Y}{100}$ |
| Temperature, T (°C) | [25,500] | (-273,+∞] | T > 25°C:<br>$T_N = 1- e^{-(aT-b)}$<br>a = 0.005<br>b = 0.125<br><br>T < 25°C:<br>$T_N = 1- e^{(aT-b)}$<br>a = 0.02<br>b = 0.5 |
| HTPI and TTP (mg/kg) | [300,4000] | [0,+∞) | $\Psi^{S}_{k,l,N} = 1 - \frac{(Score)_{k,l}}{<(Score)>_l + 2\sigma_l}$ |
| HTPE (mg/m$^3$) | [10,70] | | |
| ATP (mg/L) | [10,80] | | |
| GWP | [1,300] | [0,+∞) | $\Psi^{S}_{k,l,N} = \frac{(Score)_{k,l}}{< (Score) >_l + 2\sigma_l}$ |
| ODP | - | | |
| PCOP | [0.1,1] | | |
| AP | [0.5,2] | | |

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Nomenclature for Table 1

| | |
|---|---|
| $TOX_N$ | Normalized Value for Toxicity Parameter |
| $R_N$ | Normalized Value for Reactivity Parameter |
| $E_N$ | Normalized Value for Explosiveness Parameter |
| $F_N$ | Normalized Value for Flammability Parameter |
| $\Delta HR_N$ | Normalized Value for Heat of Reaction Parameter |
| $P_N$ | Normalized Value for Pressure Parameter |
| $Y_N$ | Normalized Value for Process Yield Parameter |
| $T_N$ | Normalized Value for Temperature Parameter |
| $\Psi^{S}_{k,l,N}$ | Normalized Value for Health and Environmental Aspects Parameter |
| $(Score)_{k,l}$ | Relative Score of Chemicals Within Impact |
| $< (Score) >_l$ | Arithmetic Average of the Score of All Chemicals Within Impact |
| $\sigma_l$ | Standard Deviation of All the Chemical Scores in Impact |
| HTPI | Human Toxicity Potential by Ingestion |
| TTP | Terrestrial Toxicity Potential |
| HTPE | Human Toxicity Potential by Inhalation or Dermal Exposure |
| ATP | Aquatic Toxicity Potential |
| GWP | Global Warming Potential |
| ODP | Ozone Depletion Potential |
| PCOP | Photochemical Oxidation Potential |
| AP | Acidification Ptential |

### 3.2 SHE Assessment Using Inherent Chemical Process Properties Data

In this study, the assessment for all three criteria of sustainability which are Inherent Chemical Safety Hazard, Inherent Chemical Health Hazard and Inherent Chemical Environmental Hazard is performed based on the index score according to Tables 3 and 5 for Inherent Chemical Safety Hazard evaluation and Inherent Chemical Health Hazard evaluation respectively.[5]. As for Inherent Chemical Safety Hazard evaluation Eq. (4) was used instead of a tabulated scores.

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***Inherent Chemical Safety Hazard***

For the evaluation of inherent chemical safety hazard, Inherent Safety Index (ISI) [16] is taken as a basis. Four parameters are taken into consideration in assessing inherent chemical safety hazard which are flammability ($I_{FL}$), explosiveness ($I_{EX}$), acute toxicity ($I_{TOX}$) and reactivity ($I_{INT}$). Table 2 shows the chemical properties that will be evaluated for each parameters and the score assignments for Inherent Chemical Safety Hazard as proposed by the ISI method [16]. The reason the scores are not standardised to a single value is due to the factors used for score formation. As an example, each parameter has different type and amount of score formation as shown in Table 2. In Table 2, flammability parameter has five score formation with scores from 0 to 4. This shows that there are five characteristics of inherent safety for flammability parameter that needs to be considered. However for toxic exposure parameter, seven score formation for seven characteristics of threshold limit value (TLV) need to be considered with scores ranging from 0 to 6. Thus, in this method the scores will be normalized for every parameter in order to produce a more standardized final assessment value. The maximum score of each parameter will then be added together as shown in Eq.(2), which resulted in the inherent chemical safety index. A lower index value represents an inherently safer process based on chemical safety properties.

$$\text{Inherent Chemical Safety Index} = (I_{FL} + I_{EX} + I_{TOX})_{max} + I_{INT,max} \quad (2)$$

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**Table 2:** Chemical Property and Score Assignments for Chemical Inherent Safety Index [5]

| Parameter | Symbol | Chemical Property | Score Formation | Score |
|---|---|---|---|---|
| Flammability | $I_{FL}$ | Flash Point | Non Flammable | 0 |
| | | | Combustible (Flash Point > 55°C) | 1 |
| | | | Flammable (Flash Point ≤ 55°C) | 2 |
| | | | Easily Flammable (Flash Point < 21 °C) | 3 |
| | | | Very Flammable (Flash Point < 0°C and boiling point ≤ 35°C) | 4 |
| Explosiveness (UEL-LEL,vol%) | $I_{EX}$ | Upper Explosive Limit – Lower Explosiveness Limit | Non Explosive | 0 |
| | | | 0 - 20 | 1 |
| | | | 20 - 45 | 2 |
| | | | 45 - 70 | 3 |
| | | | 70 - 100 | 4 |
| Toxic Exposure (ppm) | $I_{TOX}$ | TLV-STEL | TLV > 10000 | 0 |
| | | | TLV ≤ 10000 | 1 |
| | | | TLV ≤ 1000 | 2 |
| | | | TLV ≤ 100 | 3 |
| | | | TLV ≤ 10 | 4 |
| | | | TLV ≤ 1 | 5 |
| | | | TLV ≤ 0.1 | 6 |
| Reactivity | $I_{INT}$ | Chemical Interaction | Heat Formation | 1 – 3 |
| | | | Fire | 4 |
| | | | Formation of harmless, non-flammable gas | 1 |

| | | | | |
|---|---|---|---|---|
| | | | Formation of toxic gas | 2 – 3 |
| | | | Formation of flammable gas | 2 – 3 |
| | | | Explosion | 4 |
| | | | Rapid polymerisation | 2 – 3 |
| | | | Soluble toxic chemicals | 1 |

***Inherent Chemical Health Hazard***

In inherent chemical health hazard, the Inherent Occupational Health Index (IOHI) is used as the score reference [17]. There are also four parameters evaluated in assessing the inherent chemical health hazard. The four parameters are material state ($I_{MS,max}$), volatility ($I_{V,max}$), chronic toxicity ($I_{EL,max}$) and adverse health impact ($I_{R,max}$). For material state the natural form or phase of a chemical is taken into consideration whether it is in liquid, gas or solid form. Boiling point of each chemical is the property used for the volatility parameter while the eight hours exposure limit (OEL) of each chemical is used for chronic toxicity evaluation. The last parameter is the adverse health impact. Table 3 summarize the parameters and their chemical properties for inherent chemical health hazard evaluation. Taking the maximum score value for each parameters, the inherent chemical health index can be calculated using Eq.(3). A lower index value indicates a low inherent health hazard level of a process.

$$\text{Inherent Chemical Health Index} = I_{MS,max} + I_{V,max} + I_{EL,max} + I_{R,max} \quad (3)$$

**Table 3:** Chemical Property and Score Assignment for Chemical Inherent Occupational Health Index [5]

| Parameter | Symbol | Chemical Property | Score Formation | Score |
|---|---|---|---|---|
| Material State | $I_{MS}$ | Gas, Liquid, Solid | Gas | 1 |
| | | | Liquid | 2 |
| | | | Solid | 3 |
| Volatility | $I_V$ | Boiling Point | Liquid and Gas | |
| | | | Very low volatility (boiling point > 150°C) | 0 |
| | | | Low (150°C ≥ boiling point > 50°C) | 1 |
| | | | Medium (50°C ≥ boiling point > 0°C) | 2 |
| | | | High ( boiling point ≤ 0°C) | 3 |
| | | | Solid | |
| | | | Non-dusty solids | 0 |
| | | | Pellet-like, non-friable solids | 1 |
| | | | Crystalline, granular solids | 2 |
| | | | Fine, light powders | 3 |
| Chronic Toxicity | $I_{EL}$ | 8-hr OEL | Vapor (ppm) | |
| | | | OEL > 1000 | 0 |
| | | | OEL ≤ 1000 | 1 |
| | | | OEL ≤ 100 | 2 |

| | | | | |
|---|---|---|---|---|
| | | | OEL ≤ 10 | 3 |
| | | | OEL ≤ 1 | 4 |
| | | | Solid (mg/m$^3$) | |
| | | | OEL > 10 | 0 |
| | | | OEL ≤ 10 | 1 |
| | | | OEL ≤ 1 | 2 |
| | | | OEL ≤ 0.1 | 3 |
| | | | OEL ≤ 0.01 | 4 |
| Adverse Impact (R-phrase) | $I_R$ | R-phrase | Acute | |
| | | | No acute toxicity effect | 0 |
| | | | R36, R37, R38, R67 | 1 |
| | | | R20, R21, R22, R65 | 2 |
| | | | R23, R24, R25, R29, R31, R41, R42, R43 | 3 |
| | | | R26, R27, R28, R32, R34, R35 | 4 |
| | | | Chronic | |
| | | | No chronic toxicity effect | 0 |
| | | | R66 | 1 |
| | | | R33, R68/20/21/22 | 2 |
| | | | R62, R63, R39/23/24/25, R48/20/21/22 | 3 |
| | | | R40, R60, R61, R64, R39/26/27/28, R48/23/24/25 | 4 |
| | | | R45, R46, R49 | 5 |

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***Inherent Chemical Environmental Hazard***

Evaluation of inherent chemical environmental hazard requires more complicated calculations compared to the scores for inherent chemical safety and inherent health indices as shown in Table 2 and 3. Most of the existing environmental hazard evaluation involves complex score calculations with utilisation of huge amount of information [5]. Thus, in order to make the evaluation simpler and suitable for the early design stage the inherent chemical environmental index presented in this paper will only involves chemical toxicity data. Atmospheric toxicity, aquatic toxicity and terrestrial toxicity are the three parameters considered in the evaluation of inherent chemical environmental hazard based on LC50 inhalation, LC50 aquatic and LD50 values of the chemicals. According to Allen *et al*. [18], toxicity potential for a chemical is the inverse of the acute toxicity limit value. The inherent chemical environmental index is calculated by Eq.(4). Like the other two indexes, a lower value of inherent chemical environmental index indicates a lower chemical environmental hazard.

$$Inherent\ Chemical\ Environmental\ Index = \frac{1}{LC50\ inhalation} + \frac{1}{LC50\ aquatic} + \frac{1}{LD50} \quad (4)$$

***Weighing Factor***

In this case study, safety is prioritized over health and environmental indicators. The weighing score assigned for safety indicator is 0.4 and the same score 0.3 is assigned for health indicator and environmental indicator.

**3.3 GROSS PROFIT EVALUATION**

Besides evaluating both chemical routes with safety, health and environmental aspects, economic assessment is also needed. In this case study, economic assessment is made based on the gross profit estimated for both routes. Gross profit is defined as the income derived from the products sales minus the cost of raw materials [19] as written in Eq. (5).

Gross Profit = Product Sales – Raw Material Cost (5)

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### 3.4 ROUTES FOR FERTILIZER PRODUCTION

Two chemical routes for fertilizer production had been chosen for SHEE assessment in this case study. The first route is the production of ammonium nitrate from nitric acid and ammonia, while the production of ammonium sulphate fertilizer from ammonia and sulphuric acid is chosen as the second route.

- Production of Ammonium Nitrate Fertilizer
  $HNO_3$ (aq) + $NH_3$ (l) $\rightarrow$ $NH_4NO_3$ (aq)

- Production of Ammonium Sulphate Fertilizer
  $2NH_3$ (l) + $H_2SO_4$ (l) $\rightarrow$ $(NH_4)_2SO_4$ (s)

Material properties data obtained from Material Safety Data Sheet (MSDS) was used for index calculation in the assessment.

### 4.0 RESULTS AND DISCUSSION

Table 4 shows the results using the Inherent Chemical Process Properties Data while Table 7 shows the results using the Inherent Benign-ness Index (IBI).

Results produced using the Inherent Chemical Process Properties Data method are in the form of index score. A lower score value indicates the most inherently safer route. The route for ammonium nitrate production achieve a lower score value which is 2.2615 compared to the ammonium sulphate production route with 3.8448. The result suggests that the production of ammonium nitrate is inherently safer as opposed to the production of ammonium sulphate.

**Table 4:** Sustainability Index Using Inherent Chemical Process Properties Data

| Index Item | Index Score | |
|---|---|---|
| | **Ammonium Nitrate Production** | **Ammonium Sulphate Production** |
| Inherent Chemical Safety Index | 1.2 | 1.2 |
| Inherent Chemical Health Index | 0.975 | 0.975 |
| Inherent Chemical Environmental Index | 0.08649 | 1.6698 |
| **Total Score** | **2.2615** | **3.8448** |

Table 5 summarizes the individual score of each parameter for all chemicals in both chemical routes. Inherent Chemical Health Index value is the same for both routes with the index value of 13. This shows that both routes possess the same hazard level in term of health. However, there are slight differences in Inherent Chemical Safety Index score value. The route for ammonium nitrate production has lower score for Inherent Chemical Safety Index which is 11 compared to the route for ammonium sulphate production which is 12. This is due to reactivity score value for nitric acid and sulphuric acid as indicated in Table 5. Sulphuric acid has higher reactivity compared to nitric acid, which makes sulphuric acid more unstable than nitric acid. Substance that is unstable can bring more hazards compared to the stable substance.

However, there are several differences between the two routes in terms of environmental aspect. Evaluation for environmental aspect differs from the safety and health evaluation. Index for every parameters in this aspect is calculated by using Eq (3), producing the Inherent Chemical Environmental Index. Then chemicals with the highest value of Inherent Chemical Environmental Index in the route is chosen as a representation to the hazards posed by the route.

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The highest value of index indicates the maximum hazards or also known as the 'worst case' that would occur in the process. Chemical route for ammonium sulphate production has significantly higher index value compared to ammonium nitrate production which are 5.5660 and 0.2883. From Table 5, it can be seen that sulphuric acid is toxic to the environment which can also cause harm to human being through inhalation as indicated from the score value of sulphuric acid for $LC_{50}$ (Inhalation) evaluation. Although ammonium sulphate is not toxic, it may cause irritation to respiration system when inhaled hence contributing to the high score value for $LC_{50}$ index which is 5.5556.

**Table 5:** Individual Score of Each Parameters for Every Chemicals in Both Chemical Routes based on Inherent Chemical Process Properties Data Method

| Parameters | Ammonium Nitrate Production | | Ammonium Sulfate Production | |
|---|---|---|---|---|
| | **Chemicals** | **Score** | **Chemicals** | **Score** |
| **Inherent Chemical Safety Index** | | | | |
| Flammability | Nitric Acid ($HNO_3$) | 0 | Ammonia ($NH_3$) | 3 |
| | Ammonia ($NH_3$) | 3 | Sulphuric Acid ($H_2SO_4$) | 0 |
| | Ammonium Nitrate ($NH_4NO_3$) | 1 | Ammonium Sulphate $(NH_4)_2SO_4$ | 0 |
| **$I_{FL}$** | | **3** | | **3** |
| Explosiveness | Nitric Acid ($HNO_3$) | 0 | Ammonia ($NH_3$) | 2 |
| | Ammonia ($NH_3$) | 2 | Sulphuric Acid ($H_2SO_4$) | 0 |
| | Ammonium Nitrate | 0 | Ammonium Sulphate | 0 |

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| | | | | |
|---|---|---|---|---|
| | ($NH_4NO_3$) | | ($(NH_4)_2SO_4$) | |
| **$I_{EX}$** | | **2** | | **2** |
| Toxic Exposure | Nitric Acid ($HNO_3$) | 4 | Ammonia ($NH_3$) | 3 |
| | Ammonia ($NH_3$) | 3 | Sulphuric Acid ($H_2SO_4$) | 1 |
| | Ammonium Nitrate ($NH_4NO_3$) | | Ammonium Sulphate ($(NH_4)_2SO_4$) | 0 |
| **$I_{TOX}$** | | **4** | | **3** |
| Reactivity | Nitric Acid ($HNO_3$) | 3 | Ammonia ($NH_3$) | 3 |
| | Ammonia ($NH_3$) | 3 | Sulphuric Acid ($H_2SO_4$) | 4 |
| | Ammonium Nitrate ($NH_4NO_3$) | 3 | Ammonium Sulphate ($(NH_4)_2SO_4$) | 3 |
| **$I_{INT}$** | | **3** | | **4** |
| **Inherent Chemical Safety Index** | | **12** | | **12** |
| **Inherent Occupational Health Index** | | | | |
| Material State | Nitric Acid ($HNO_3$) | 2 | Ammonia ($NH_3$) | 2 |
| | Ammonia ($NH_3$) | 2 | Sulphuric Acid ($H_2SO_4$) | 2 |
| | Ammonium Nitrate ($NH_4NO_3$) | 3 | Ammonium Sulphate ($(NH_4)_2SO_4$) | 3 |
| **$I_{MS}$** | | **3** | | **3** |

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| | | | | |
|---|---|---|---|---|
| Volatility | Nitric Acid ($HNO_3$) | 1 | Ammonia ($NH_3$) | 3 |
| | Ammonia ($NH_3$) | 3 | Sulphuric Acid ($H_2SO_4$) | 0 |
| | Ammonium Nitrate ($NH_4NO_3$) | 2 | Ammonium Sulphate $(NH_4)_2SO_4$ | 2 |
| **$I_V$** | | **3** | | **3** |
| Chronic Toxicity | Nitric Acid ($HNO_3$) | 3 | Ammonia ($NH_3$) | 2 |
| | Ammonia ($NH_3$) | 2 | Sulphuric Acid ($H_2SO_4$) | 3 |
| | Ammonium Nitrate ($NH_4NO_3$) | 1 | Ammonium Sulphate $(NH_4)_2SO_4$ | 1 |
| **$I_{EL}$** | | **3** | | **3** |
| Adverse Impact | Nitric Acid ($HNO_3$) | 4 | Ammonia ($NH_3$) | 4 |
| | Ammonia ($NH_3$) | 4 | Sulphuric Acid ($H_2SO_4$) | 4 |
| | Ammonium Nitrate ($NH_4NO_3$) | 3 | Ammonium Sulphate $(NH_4)_2SO_4$ | 4 |
| **$I_R$** | | **4** | | **4** |
| **Inherent Chemical Health Index** | | **13** | | **13** |
| **Inherent Chemical Environmental Index** | | | | |
| $LC_{50}$ | Nitric Acid | 0.0149 | Ammonia | 0.0005 |

| | | | | |
|---|---|---|---|---|
| (Inhalation) | ($HNO_3$) | | ($NH_3$) | |
| | Ammonia ($NH_3$) | 0.0005 | Sulphuric Acid ($H_2SO_4$) | 1.9608 |
| | Ammonium Nitrate ($NH_4NO_3$) | 0.0112 | Ammonium Sulphate $(NH_4)_2SO_4$ | 5.5556 |
| $LC_{50}$ (Aquatic) | Nitric Acid ($HNO_3$) | 0.0139 | Ammonia ($NH_3$) | 0.2849 |
| | Ammonia ($NH_3$) | 0.2849 | Sulphuric Acid ($H_2SO_4$) | 0.0102 |
| | Ammonium Nitrate ($NH_4NO_3$) | 0.0007 | Ammonium Sulphate $(NH_4)_2SO_4$ | 0.01 |
| $LD_{50}$ | Nitric Acid ($HNO_3$) | 0.0111 | Ammonia ($NH_3$) | 0.0029 |
| | Ammonia ($NH_3$) | 0.0029 | Sulphuric Acid ($H_2SO_4$) | 0.00047 |
| | Ammonium Nitrate ($NH_4NO_3$) | 0.0005 | Ammonium Sulphate $(NH_4)_2SO_4$ | 0.00035 |
| **Inherent Chemical Environmental Index** | | **0.2883** | | **5.5660** |

Meanwhile, the scores calculated previously are normalized and weighing factor is assigned for each criteria. Normalization was done by dividing the calculated score with the score range in order to produce results with the same magnitude. The purpose of this step is to ensure that all values are comparable. This case study prioritizes safety aspects above the environmental and health aspects. Table 6 shows the score and weighing factor given to every index. The total

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index score shows that the chemical route for ammonium nitrate production is inherently more benign than the chemical route for ammonium sulphate production.

**Table 6:** Index Score and Weighing Factor for Inherent Chemical Process Properties Data Method

| Index | Normalized Value | Weighing Factor | Score | Normalized Value | Weighin g Factor | Score |
|---|---|---|---|---|---|---|
| | Ammonium Nitrate | | | Ammonium Sulphate | | |
| Inherent Chemical Safety Index | 3 | 0.4 | 1.2 | 3 | 0.4 | 1.2 |
| Inherent Chemical Health Index | 3.25 | 0.3 | 0.975 | 3.25 | 0.3 | 0.975 |
| Inherent Chemical Environmental Index | 0.2883 | 0.3 | 0.0864 9 | 5.5660 | 0.3 | 1.6698 |
| **Total Index Score** | | | **2.2615** | | | **3.8448** |

The same assessment was then conducted on the same chemical routes using the IBI method. There are three main indicators assessed which are safety, health and environment. In this assessment, safety aspect is divided into two sub-indicators which are chemical safety aspect and process safety aspect. Both chemical safety aspect and process safety aspect consists of four parameters each. Toxicity, reactivity, explosiveness and flammability are the parameters for chemical safety aspect. In process safety aspect the four parameters are heat of reaction,

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pressure, process yield and temperature. Human Toxicity Potential by Ingestion (HTPI), Terrestrial Toxicity Potential (TTP), Human Toxicity Potential by Inhalation (HTPE) and Aquatic Toxicity Potential (ATP) are the parameters evaluated in health aspect. Table 7 shows all the parameters evaluated as well as its normalized score. Evaluation on chemical safety, process safety and health aspect are done by using data obtained in MSDS and scoring methods obtained from Table 1. However, in order to obtain data for Global Warming Potential (GWP), Acidification Potential (AP), Photochemical Ozone Creation Potential (PCOP) and Ozone Depletion Potential (ODP) in environmental aspect, WAR GUI software was used. A lower Cumulative Index (CI) value indicates an inherently safer chemical route. Calculated results from Table 7 shows that chemical route for the production of ammonium nitrate has lower Cumulative Index (CI) value of 6.2893 compared to the ammonium sulphate production which is 6.4499.

Sustainability assessment by using the IBI agrees with the assessment result by using the Inherent Chemical Process Properties Data, that the chemical route of ammonium nitrate production is inherently more benign than the chemical route for ammonium sulphate production.

Economic evaluation based on gross profit shows that the production of ammonium nitrate is more profitable than the production of ammonium sulphate. This evaluation resulted in 0.05 US Dollar profit for every pound of ammonium nitrate sold compared to 0.0013 US Dollar profit for every pound of ammonium sulphate sold. This might be due to the lower selling price of ammonium sulphate which is 0.14 US Dollar for every pound compared to ammonium nitrate which is 0.26 US Dollar for every pound.

**Table 7:** Results Produced by Using the Inherent Benign-ness Index (IBI)

| Parameter Involved | Normalized Score | |
|---|---|---|
| | **Production of Ammonium Nitrate** | **Production of Ammonium Sulfate** |
| **Chemical Safety Aspect** | | |
| Toxicity | 1 | 0.75 |
| Reactivity | 0 | 0.5 |
| Explosiveness | 0.13 | 0.13 |
| Flammability | 0.5 | 0.25 |
| **Process Safety Aspect** | | |
| Heat of Reaction | 0.4865 | 0.9733 |
| Pressure | 0.0833 | 0.0861 |
| Process Yield | 0.0526 | 0.0526 |
| Temperature | 0.4908 | 0.1605 |
| **Health Aspect** | | |
| HTPI | 0.7625 | 0.7632 |
| TTP | 0.7625 | 0.7632 |
| HTPE | 0.9963 | 0.9963 |
| ATP | 0.1975 | 0.1974 |
| **Environmental Aspect** | | |
| GWP | 0.0259 | 0.0259 |
| ODP | $2.7266 \times 10^{-7}$ | $2.716 \times 10^{-7}$ |
| PCOP | $9.4749 \times 10^{-6}$ | $9.4724 \times {}^{-6}$ |
| AP | 0.8014 | 0.8014 |
| **Cumulative Index (CI)** | **6.2893** | **6.4499** |

**5.0 CONCLUSION**

In this study, SHE (safety, health and environmental) assessments was performed for production of ammonium nitrate and ammonium sulphate using two different assessment, Inherent Benign-ness Index (IBI) and Inherent Chemical Process Properties Data. It was found that both methods agree with each other that the chemical route for ammonium nitrate is safer than the ammonium sulphate for the production of fertilizer. Both methods requires data from Material Safety Data Sheet only and therefore, are suitable for application during process design stage with very much data lacking. There are also indicators in Inherent Benign-ness Index (IBI) that does not exist in Inherent Chemical Process Properties Data which are the evaluation of safety in terms of operating process. These details adds more complexity in the assessment conducted. Although the route is favorable in term of SHE aspects, however economic aspect cannot be ignored. Thus, evaluation of economic aspect using gross profit analysis is conducted in this study. The results highlighted that ammonium nitrate production route provides the most attractive gross profit.

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