

# COST EFFECTIVE INHERENT SAFETY INDEX FOR PROTON EXCHANGE MEMBRANE FUEL CELL SYSTEMS

Nordin, Nazatul Niza<sup>1</sup>, Ahmad, Arshad<sup>2</sup>, Mohamad, Mardawani<sup>2</sup> and Ali, Mohamad Wijayanuddin<sup>2,\*</sup>

<sup>1</sup>IKIP International College, 25050 Kuantan, Pahang, Malaysia

E-mail: nazatulniza@ikip.edu.my

<sup>2</sup>Institute of Hydrogen Economy, Faculty of Chemical Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia

E-mail: m.w.ali@cheme.utm.my

\*Corresponding author

## ABSTRACT

There have been many indices available in the process industries to describe, rank or quantify hazards to people, properties and environments. Most of the developed methods were meant to be applied to large scale and complex systems of process industries. Development of a swift and simple inherent safety index method which is relevant to small scale, less complex membrane fuel cell system particularly the one in which to be applied during an early design stage is essential as an alternative to current comprehensive and yet time-consuming indices. In this work, a modified version of PIIS, modified prototype index for inherent safety (*m*-PIIS) was developed with the objectives of identifying, indicating and estimating inherent safety of fuel cell system at an early design stage. The developed index was tested at four proton exchange membrane (PEM) fuel cell systems namely high pressure PEMFC system, low pressure PEMFC system, LH<sub>2</sub> PEMFC system and on-board Me-OH PEMFC system. The developed index was also benchmarked against the original PIIS and ISI using the published results for the selection of process routes in MMA production. Results have indicated that *m*-PIIS has strong positive relationship with PIIS and ISI on most of the reaction step in MMA with the most significant are the C<sub>4</sub>, TBA, and C<sub>3</sub> reaction steps. Other reaction steps such as C<sub>2</sub>/MP, C<sub>2</sub>/PA and ACH showed a strong positive relationship as well.

## NOMENCLATURE

|                  |                                |
|------------------|--------------------------------|
| F                | Flammability scores            |
| I <sub>CI</sub>  | Chemical Inherent Safety Index |
| I <sub>ISI</sub> | Inherent Safety Index          |
| I <sub>PI</sub>  | Process Inherent Safety Index  |
| K <sub>C</sub>   | Chemical Index                 |
| K <sub>P</sub>   | Process Index                  |
| P                | Pressure score                 |
| S <sub>EQ</sub>  | Equipment safety score         |
| T                | Temperature score              |
| X                | Explosiveness scores           |
| T <sub>x</sub>   | Toxicity                       |

## 1.0 INTRODUCTION

The possibility of replacing the internal combustion engine used in road vehicles with more efficient, low emission, alternative power sources has been considered since 1960s. Among the various renewable energy sources, fuel cell is gaining more popularity due to their higher efficiency, cleanliness and cost-effective supply of power demanded by the consumers. The remarkable features of fuel cell such as continuous operation (no recharging), relatively low operating temperature, high power density, as well as low or zero emission (when operating on hydrogen) and easy scale-up makes proton exchange membrane

fuel cell (PEMFC) a suitable candidate to be the next generation power sources for transportation, stationary, and portable applications. The simplest and most practical PEMFC systems for powering a car are those where fuel is converted directly to electricity such as direct-hydrogen or direct methanol PEMFC.

A fuel cell vehicle is a motor vehicle having a fuel cell engine as its prime mover. Among the main obstacles in introducing fuel cell vehicles are the acceptability of hydrogen as a fuel and the lack of a suitable storage medium for hydrogen on-board vehicle. With respect to the former, there is some concern over safety when using hydrogen. Indeed as a fuel, hydrogen does create certain risks due to its unique handling requirements, as compared to other alternative fuels. It has minimum ignition energy lower than that of other hydrocarbon fuels and a much wider flammability range. Furthermore, hydrogen storage methods are different from storage methods for other fuels. One of the main safety concerns is the safety for onboard storage of hydrogen in transportation.

## **2.0 INHERENT SAFETY**

Inherent safety (originally known as intrinsic safety) as a concept was promulgated by Trevor Kletz in the late 1970s and is based on common sense, which includes avoiding use of hazardous materials, minimising the inventories of hazardous materials and aiming for simpler processes with more benign and moderate process alternatives. An inherent safety process avoids hazards instead of creating situations that will lead to hazards and then trying to control it. Major principles of inherent safety approaches integrated into the inherently safer design are minimise (intensify), reduction in the quantity of hazardous materials, substitute or replace hazardous materials with safer materials, attenuate (moderate), use or operate materials in a less hazardous form or conditions and, simplify and avoid unnecessary complexity in facilities and processes.

A chemical process can have multiple hazards associated with it. Hazards may arise due to raw materials, intermediates, final products, side and waste products, the nature of the process, the mode of operation, the complexity of the process steps, environmental conditions and others. A process goes through various stages of evolution, including research, process development, design, construction, operation, maintenance, modifications and finally decommissioning. [1] Of all the stages, inherent safety is best considered during the initial stages of design, when the choice of process route and concept is made. [2,3]

### **2.1. Inherent Safety Index**

In the early 1990s, several process safety evaluation methods were already existed such as Dow and Mond Index and HAZOP studies. Unfortunately, they were not directly suitable to be used as analysis tools in preliminary process design. Most of the methods require too detailed process information and were not directly applicable. [4] A large variety of methods were used to identify and assess hazard potential of chemical processes during the design phase. These methods vary significantly in goal, scope, structure and the exact way of considering safety aspects. Some index-based methods have been developed applying the concept of inherent safety and considering the limited amount of information at early design stages.

Many of the proposed methods are very elegant, yet too involved for easy adoption by the industry which is scared of yet another safety analysis regime. [5] In a survey by Gupta and Edwards (2002), [6] companies desired a rather simple method to measure inherent safety during design. Simplification is an important characteristic of inherent safety. It is therefore desirable to have a simple inherent safety procedure.

## 2.2. Prototype Index of Inherent Safety (PIIS)

Edwards and Lawrence, 1993 [7] have made one of the first attempt to develop an indexing methodology to incorporate inherent safety in the design procedure. Prototype Index of Inherent Safety (PIIS) was the first index published for evaluating the inherent safety in process pre-design. It is intended for analysing the choice of process route, i.e. the raw materials used and the sequence of the reaction steps based on seven important parameters. This method is reaction-step oriented, and it does not consider much the other parts of the process. The PIIS is calculated as a total score, which is a sum of a Chemical Score and a Process Score. The Chemical Score consists of inventory, flammability, explosiveness and toxicity. The Process Score includes temperature, pressure and yield. The PIIS has some clear advantages over some other numerical indices in early design stages, because it can be used when most of the detailed process information is still lacking.

$$PIIS = \sum \text{Chemical score} + \text{Process score} \quad (1)$$

## 2.3. Inherent Safety Index (ISI)

Inherent Safety Index (ISI) was developed by Heikkila, 1999 [2] to take into consideration a larger scope of process steps. It is not only considering the reaction route but also the separation sections as well. ISI is based on the evaluation of twelve parameters, which are selected to represent major inherent safety factors and are already available in the conceptual design phase. ISI consists of two main index groups. The Chemical Inherent Safety Index ( $I_{CI}$ ) describes the chemical aspects of inherent safety and the Process Inherent Safety Index ( $I_{PI}$ ) represents the process related aspects. Inherent Safety Index ( $I_{ISI}$ ) is a sum of the chemical inherent safety index ( $I_{CI}$ ) and the process inherent safety index ( $I_{PI}$ ).

$$I_{ISI} = I_{CI} + I_{PI} \quad (2)$$

## 2.4. Other Inherent Safety Indices

i-Safe index [1] was developed as an intelligent design support system for performing inherent safety analysis during early stages of design. It identifies the hazards that are associated with the reactions and the chemicals involved in the process route and rank the available process routes for the product chosen in the product specification stage. The index compares process routes by using sub-indices values obtained from ISI and PIIS with additional NFPA reactivity rating values for the chemicals present. Information used for analysis are reaction conditions, materials involved, heat of reaction, catalysts, phase of reaction, unit process involved, and process yield. Gentile et. al., (2003) [8] attempted to improve some of the subjective factors in the inherent safety index of Heikkila, (1999) [2] by using fuzzy set theory. The alterations were aimed at improving the (excessiveness or insufficient) sensitivity in the ranges selected for each of the various index parameters. The fuzzy logic system was applied for the calculation of proposed inherent safety index based on 'if-then' rules that describe knowledge related to inherent safety. Each factor is described by a linguistic variable whose range of interest is divided into fuzzy sets. For each set, a membership function is defined which has a specific shape describing the physical behaviour of the set.

### 3.0. METHODOLOGY

*m*-PIIS is developed in a sequence of steps according to the outlined flowchart as shown in Fig.1.

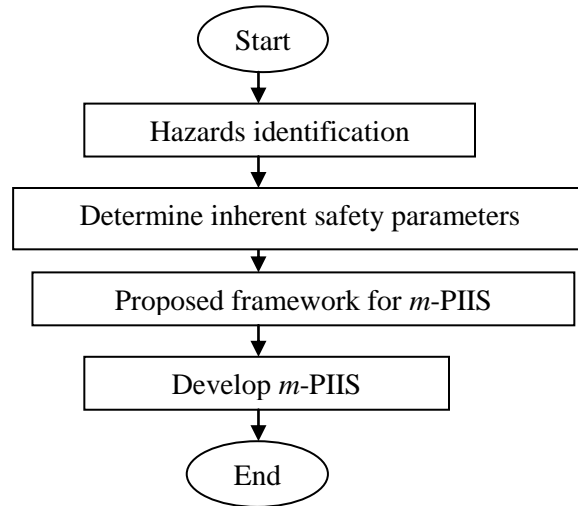


Figure 1. Flowchart showing steps in the development of *m*-PIIS

The first important part of any assessment method is a clear definition of its goal and scope. [9] This severity index is designed to indicate and estimate the level of inherent safety of two types of PEM fuel cell system configurations utilised in fuel cell vehicles; direct hydrogen fuel cell system and direct methanol fuel cell system. The index will be developed based on the probability of the occurrence of the hazards only and shall not include the consequences of the hazards. It is intended to act as a guide and should be sufficed to estimate inherent danger. Framework for the development of *m*-PIIS shall take into account the original framework set by PIIS. Modifications should be made to the existing PIIS to satisfy the less complex nature of the system investigated and for the purpose of developing a swift and simple index applicable at early design stage.

Hazards of the hydrogen fuel cell system are determined from previous literature and material safety datasheets. Hazards identification and risk assessment studies can be performed at any stage during the initial design or ongoing operation of a process. Hazard identification can be performed independent of risk assessment. [10] Inherent safety parameters of the system are determined from previous literature and former indices. The framework is outlined based on the defined goal, hazards and inherent safety parameters of the system. The index (*m*-PIIS) is modified from PIIS therefore the framework for this index is mainly derived from the original work of Edwards and Lawrence, (1993). [7] Outcome of the development are further discussed in later section.

#### 3.1. Case Study

Four PEM hydrogen fuel cell system configurations were selected as the case studies. The *m*-PIIS index is tested on the following hydrogen fuel cell configurations.

##### 3.1.1. High Pressure PEMFC System (Chevrolet Equinox Fuel Cell)

The Chevrolet Equinox is the General Motor's fourth generation fuel cell vehicle (a five-door front wheel drive SUV). It incorporates a 4.2 kg, 700 bar compressed hydrogen gas (CGH<sub>2</sub>) storage system. For packaging reasons the storage system comprises not a single but two, respectively three (Type IV) pressure vessels. Because of the comparatively high operating pressure of these vessels, a cylindrical

design is both essential and obvious. The fuel cell system (operating life 2.5 years or 80,000 km) which operates at  $-25^{\circ}\text{C}$  to  $45^{\circ}\text{C}$  consists of 440 cells (93 kW) fuel cell stacks and a 35 kW NiMH battery. Chevrolet Equinox has an operating range of 320 km, with a maximum speed of 160 km/h and an acceleration range from 0 – 100 km/h in 12s.

### **3.1.2. Low Pressure PEMFC System (Hyundai Santa Fe)**

Hyundai Motor Company has developed hydrogen fuel cell vehicles (FCV) based on its SUV, Santa Fe. As the hydrogen fuel cell power plant runs at the low pressure, parasitic loss due to its operation is fully minimised and the noise level of the air supply subsystem is extremely low. Gaseous hydrogen is stored up to 200 bars in a tri-shield composite (Type IV) tank. The hydrogen storage density is about 7.5 wt%. The liner to contain hydrogen is seamless and made of high-density polyethylene and thus possible failure is minimised. The fuel cell power plant consists of a stack of proton exchange membrane fuel cell (operating at  $80^{\circ}\text{C}$ ) to generate electricity. The electric drive train of Santa Fe FCV consists of an inverter, an induction motor and a gear differential unit (GDU). The motor is designed to deliver power of continuous 20 kW and maximum 65 kW. Santa Fe FCV has an operating range of 160 km, with a maximum speed of 126 km/h and an acceleration range from 0 to 96.4 km/h in 17.4 s.

### **3.1.3. LH<sub>2</sub> – PEMFC System (GM HydroGen 3)**

GM HydroGen 3 Opel Zafira (a multi-purpose vehicle, MPV) is an example of adaptable vehicle, i.e., capable of using either liquid or compressed hydrogen storage type. The HydroGen 3 vehicles are currently capable of storing 68 L or 4.6 Kg H<sub>2</sub> (LH<sub>2</sub> variant). The liquid hydrogen storage tank is made of stainless steel, installed ahead of rear axle under rear seat. The corresponding PEM fuel cell system is operating at  $-253^{\circ}\text{C}$ , with cryogenic LH<sub>2</sub> storage operating at 5 – 10 bars. The fuel cell system comprises of 200 individual fuel cell stacks wired in series, with a power output of 94 kW. GM HydroGen 3 Opel Zafira has an operating range of 400 km, with a maximum speed of 160 km/h and an acceleration range from 0 to 100 km/h in 16 s. Fuel cell system of GM HydroGen 3 has been packaged in a way that it fits together with the electric traction system into the same volume as an ICE propulsion module, and can be fixed to the same mount. This allows the simple and cost efficient vehicle assembly in existing facilities.

### **3.1.4. On-board Methanol PEMFC System (Necar 5)**

DaimlerChrysler methanol-powered vehicle, Necar 5 is a five seat compact car with front-wheel drive based on the A-class of Mercedes-Benz. The A-class has a double or sandwich-floor, which offers extra space for holding non-conventional components and makes this model particularly suitable for conversion into FCEVs. The Necar 5, 75 kW fuel cell systems utilises energy from the methanol 25 percent more efficiently. The fuel cell stack is 50 percent more powerful than its predecessor in the NECAR series, with operating temperatures at 300 -  $400^{\circ}\text{C}$  and 3 bar pressure. DaimlerChrysler has chosen methanol as the source for hydrogen which they describe as a 'hydrogen storage medium in liquid form,' and have even given the alcohol a new name - "methanolised hydrogen or MH<sub>2</sub>". DaimlerChrysler Necar 5 has an operating range of more than 450 km, with a top speed of 150 km/h and an acceleration range from 0 to 100 km/h in 16 s.

## **4.0. RESULTS AND DISCUSSIONS**

### **4.1. Fuel Cell System Hazards**

For fuels, hazard is mostly due to the physical properties of the fuel i.e. any one of the properties might cause a source for hazard. Hydrogen represents a greater hazard (over methane and gasoline) due to the

wider flammability limits, lower ignition energy and higher deflagration index. It is also clearly proven that high pressure hydrogen gas is more difficult to be contained compared to liquid gasoline. [11]

Adamson, 2000 [12] compares the physical properties of hydrogen and methanol. Between hydrogen and methanol, hydrogen has the “explosive” public image and there is concern as to how the public may react to refuelling with what perceive as a very dangerous fuel. Methanol by contrast has quite a safe public image.

Therefore it can be concluded that the hazards of the fuel cell system are contributed by the fuel physical properties such as the physical state, toxicity, flammability limits, flash points and low ignition energy. Hydrogen in the form of gas is more difficult to be contained compared to liquid hydrogen. Extreme operating conditions (high and low temperature and pressure) may enhance the hazards contributed by the fuel physical properties. According to Bultel et. al., 2007 [13] fuel cell and fuel cell subsystem is also a source of hazard. Fuel cell system including reformer and other equipment utilised is a system under pressure and a source of hazard.

#### **4.2. Inherent Safety Parameters for the System**

As shown in Table 1, based on the principles of inherent safety (substitution, attenuation, limitation of effects and tolerance) as described by Heikkila, 1999 [2] and Rahman et al. (2005), [4] the inherent safety parameters were selected for the development of m-PIIS. Five out of six inherent safety parameters of m-PIIS are retained from the original PIIS, while another parameter is taken from ISI. The selected parameters are flammability, explosiveness, toxicity, temperature and pressure. Type of equipment or equipment safety is a significant parameter from ISI, introduced into m-PIIS.

Established indices such as PIIS, ISI and i-Safe took into account flammability parameter in the calculation of their index value. Explosive limits were used in PIIS, ISI and i-Safe to determine the explosiveness of chemical substance. Toxicity was selected as the parameters in the calculation of the three former indices, PIIS, ISI and i-Safe. Temperature is an ultimate credible parameter unanimously agreed by previous literature [Edwards (1993),[7] Heikkila (1996), [14] Gupta (2003), [5] Palaniappan (2004), [1] Leong and Shariff (2008, 2009) [15,16] and Landucci (2008) [17]] to demonstrate inherent safety because temperature is a direct measure of the heat energy available at release. Pressure was selected in previous literature [Edwards (1993), [7] Heikkila (1996, 1999), [2,14] Gupta (2003) [5] and Palaniappan (2004) [1]] due to its ability of measuring both the energy available at release and the energy available to cause a release.

Scores for flammability, explosiveness, temperature, and pressure and equipment safety are based on the work of Heikkila, 1996. [14] ISI adopted simpler score range which is more appropriate and applicable to represent the system under investigation. Score for the most dangerous equipment will be chosen as the indicator of the overall equipment safety level. However, score for toxicity is based on the readily available NFPA ranking. NFPA ranking will allow effortless reference thus fulfilling the main purpose of the development of this index, which is swift and easy.

#### **4.3. Development and Calculation of m-PIIS**

Calculation for modified prototype index for inherent safety (m-PIIS) is following the quantification of previous established inherent safety indices, in particular PIIS and ISI. Both PIIS and ISI computed their indices by summation of the Chemical sub-index and Process sub-index.

Table 1. Selected parameters for m-PIIS

| Inherent safety parameters | PIIS | ISI | i-Safe | m-PIIS |
|----------------------------|------|-----|--------|--------|
| Heat of reaction           |      | √   | √      |        |
| Heat of side reaction      |      | √   |        |        |
| Chemical interaction       |      | √   |        |        |
| Reactivity rating          |      |     | √      |        |
| Flammability               | √    | √   | √      | √      |
| Explosiveness              | √    | √   | √      | √      |
| Toxicity                   | √    | √   | √      | √      |
| Corrosiveness              |      | √   |        |        |
| Inventory                  | √    | √   |        |        |
| Yield                      | √    |     | √      |        |
| Temperature                | √    | √   | √      | √      |
| Pressure                   | √    | √   | √      | √      |
| Type of equipment          |      | √   |        | √      |
| Process structure          |      | √   |        |        |

#### 4.4. Chemical Index ( $K_C$ )

Chemical index consists of scores for physical properties of the chemicals including, flammability scores (F), explosiveness scores (X) and toxicity ( $T_x$ ).

$$K_c = F + X + T_x \quad (3)$$

#### 4.5. Process Index ( $K_p$ )

Process index includes temperature score (T), pressure score (P) and equipment safety score ( $S_{EQ}$ ).

$$K_p = T + P + S_{EQ} \quad (4)$$

#### 4.6. Modified Prototype Index for Inherent Safety (m-PIIS)

Modified prototype index for inherent safety (m-PIIS) is calculated as a total score of Chemical Index and Process Index.

$$m - PIIS = K_c + K_p \quad (5)$$

Calculation of m-PIIS is made on the basis of the worst case scenario. Approach employed is based on the most hazardous condition that can appear. A low index value indicates an inherently safer process, whereas a high index score indicate less safe process. Theoretically, possible ranges of Chemical Index,  $K_C$  and Process Index,  $K_p$  are between 0 and 12 and thus theoretically the m-PIIS will have a range of between 0 and 24.

Table 2 summarised the m-PIIS index value for the four case studies. For all the three fuel cell system; GM Chevrolet Equinox, Hyundai Santa Fe, GM HydroGen 3, DaimlerChrysler Nekar 5; Chemical Index ( $K_C$ ) score is almost uniform due to the fact that  $K_C$  is the measure of hazards contributed by physical properties of the fuel i.e., summation of flammability (F) score, explosiveness (X) score and toxicity ( $T_X$ ) score of the fuel used. As an addition, all the three systems are using hydrogen to feed the fuel cell system. In the case of Me-OH PEMFC (Nekar 5), both fuel methanol and hydrogen are presence as the chemical fuel, therefore the most hazardous outcome will be considered when calculating the respective Chemical Index score. For Nekar 5, toxicity ( $T_X$ ) score is assigned as 1 due to the presence of methanol which is regarded by NFPA as ‘may be irritating’ in comparison to hydrogen which is assigned by NFPA as 0 and considered as “no unusual hazard”.

Table 2. Summary of m-PIIS values for four case studies

| Fuel cell system         | Scores |   |   | $K_C$ | Scores |   |          | $K_p$ | m-PIIS |
|--------------------------|--------|---|---|-------|--------|---|----------|-------|--------|
|                          | F      | X | T |       | T      | P | $S_{EQ}$ |       |        |
| GM Chevrolet Equinox     | 4      | 4 | 0 | 8     | 1      | 4 | 3        | 8     | 16     |
| Hyundai Santa Fe         | 4      | 4 | 0 | 8     | 1      | 3 | 3        | 7     | 15     |
| GM HydroGen 3            | 4      | 4 | 0 | 8     | 1      | 1 | 3        | 5     | 13     |
| Daimler Chrysler Nekar 5 | 4      | 4 | 1 | 8     | 3      | 0 | 3        | 6     | 15     |

Process Index ( $K_p$ ) scores does show some variations because  $K_p$  is a measure of operating conditions which include operating temperature (T) score, pressure (P) score and equipment safety ( $S_{EQ}$ ) score. High or low operating conditions do impose certain level of hazards. Nekar 5 has the highest temperature (T) score since it is operating at 300 - 400°C and yet the lowest pressure (P) scores. GM Chevrolet Equinox is assigned the highest pressure (P) score because the hydrogen gas was compressed to 700 bars and does pose significant hazards. GM HydroGen 3 has the lowest index value, followed by DaimlerChrysler Nekar 5, Hyundai Santa Fe and GM Chevrolet Equinox. A low index value indicates an inherently safer process and a high index score indicate less safer process.

#### 4.7. Benchmarking of m-PIIS

The new index is benchmarked against the published results of other established indices (PIIS and ISI) based on case studies of various process routes to produce methyl methacrylate acid or MMA (Rahman et. al., 2005). [4] Methyl methacrylate is an organic compound widely used in the production of acrylic plastics and PVC. MMA can be manufactured through various process routes. The six established process routes or reaction steps are: acetone cyanohydrins (ACH) reaction step, ethylene via propionaldehyde ( $C_2/PA$ ) reaction step, ethylene via methyl propionate ( $C_2/MP$ ) reaction step, propylene ( $C_3$ ) reaction step, isobutylene, ( $C_4$ ) reaction step, and *tert*-butyl alcohol (TBA) reaction step. As previously practiced by other researchers such as PRI (Leong and Shariff, 2009), [16] HQI (Hassim and Hurme, 2010) [18] and EHI (Cave and Edwards, 1997), [19] benchmarking step is utilising MMA process. m-PIIS index values for each MMA reaction step are compared with the respective index values of PIIS and ISI as shown in Table 3 and line plots in Fig. 2 to Fig.8.



Table 3. Comparison of index values between m-PIIS, PIIS and ISI

| Reaction step                   | m-PIIS | PIIS | ISI |
|---------------------------------|--------|------|-----|
| ACH <sub>1</sub>                | 17     | 28   | 25  |
| ACH <sub>2</sub>                | 12     | 16   | 21  |
| ACH <sub>3</sub>                | 10     | 11   | 21  |
| ACH <sub>4</sub>                | 10     | 14   | 19  |
| ACH <sub>5</sub>                | 14     | 19   | 19  |
| ACH <sub>6</sub>                | 10     | 15   | 18  |
| C <sub>2</sub> /PA <sub>1</sub> | 15     | 21   | 23  |
| C <sub>2</sub> /PA <sub>2</sub> | 13     | 26   | 23  |
| C <sub>2</sub> /PA <sub>3</sub> | 13     | 16   | 21  |
| C <sub>2</sub> /PA <sub>4</sub> | 11     | 16   | 16  |
| C <sub>2</sub> /MP <sub>1</sub> | 17     | 26   | 24  |
| C <sub>2</sub> /MP <sub>2</sub> | 11     | 10   | 21  |
| C <sub>2</sub> /MP <sub>3</sub> | 12     | 26   | 17  |
| C <sub>3</sub> 1                | 16     | 24   | 27  |
| C <sub>3</sub> 2                | 10     | 12   | 22  |
| C <sub>3</sub> 3                | 10     | 15   | 18  |
| C <sub>3</sub> 4                | 9      | 16   | 16  |
| C <sub>4</sub> 1                | 13     | 17   | 20  |
| C <sub>4</sub> 2                | 13     | 17   | 21  |
| C <sub>4</sub> 3                | 9      | 16   | 16  |
| TBA <sub>1</sub>                | 10     | 15   | 20  |
| TBA <sub>2</sub>                | 13     | 17   | 21  |
| TBA <sub>3</sub>                | 9      | 15   | 16  |

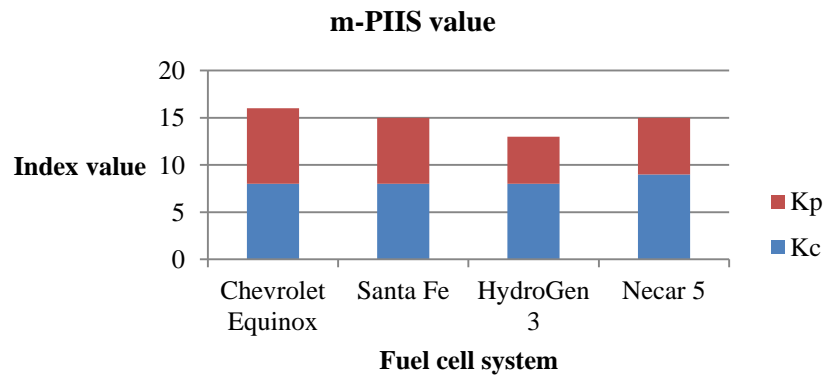


Figure 2. m-PIIS value for the fuel cell systems

Fig.3 represents the index values of m-PIIS, PIIS and ISI, calculated for acetone cyanohydrins (ACH) process route. For this reaction step, m-PIIS shows a strong positive relationship with PIIS ( $r = 0.957$ ) and ISI ( $r = 0.793$ ).

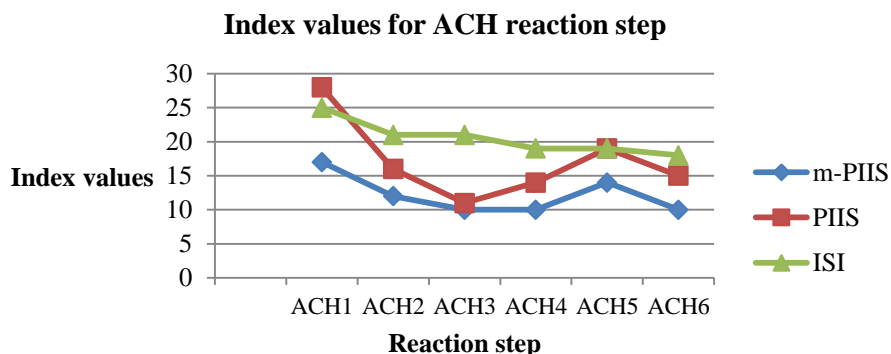


Figure 3. Comparison of index values for each ACH reaction steps

Index values for ethylene via propionaldehyde ( $C_2/PA$ ) reaction steps are shown in Fig.4. In  $C_2/PA$  reaction step, m-PIIS shows a strong relationship with ISI ( $r = 0.865$ ) but a slightly poor relationship with PIIS ( $r = 0.426$ ).

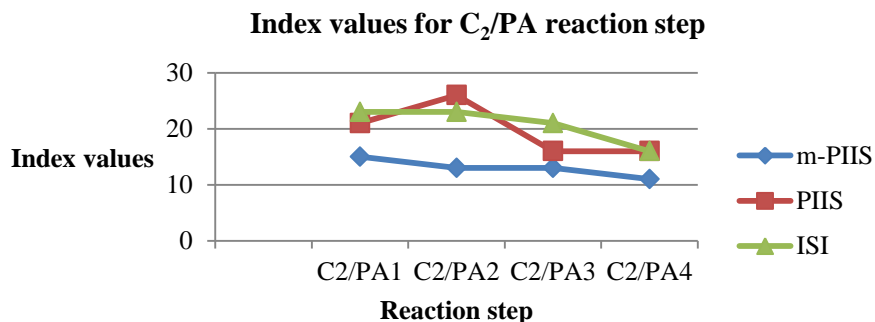


Figure 4. Comparison of index values for  $C_2/PA$  reaction steps

Fig.5 displays the line plots of index values for ethylene via methyl propionate ( $C_2/MP$ ) process routes. It shows that m-PIIS has a strong relationship with both ISI ( $r = 0.723$ ) and PIIS ( $r = 0.629$ ). An index value for propylene ( $C_3$ ) reaction routes is shown in Fig.6. It is apparent that m-PIIS shows a strong positive relationship with the two pioneered indices. m-PIIS shows a correlation value of 0.899 against PIIS and a value of 0.906 against ISI.

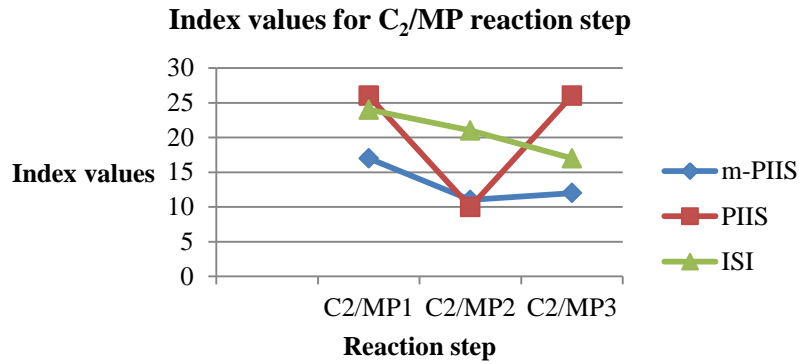


Figure 5. Comparison of index values for C<sub>2</sub>/MP reaction steps

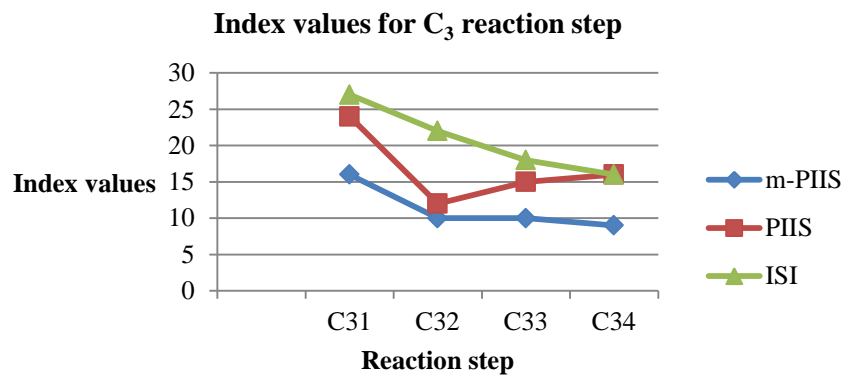


Figure 6. Comparison of index values for C<sub>3</sub> reaction steps

Fig.7 shows the line plots indicating the index values of isobutylene (C<sub>4</sub>) reaction step. Clearly evidenced that m-PIIS shows a significant strong positive relationship with PIIS ( $r = 1.000$ ) and ISI ( $r = 0.982$ ) for C<sub>4</sub> reaction step.

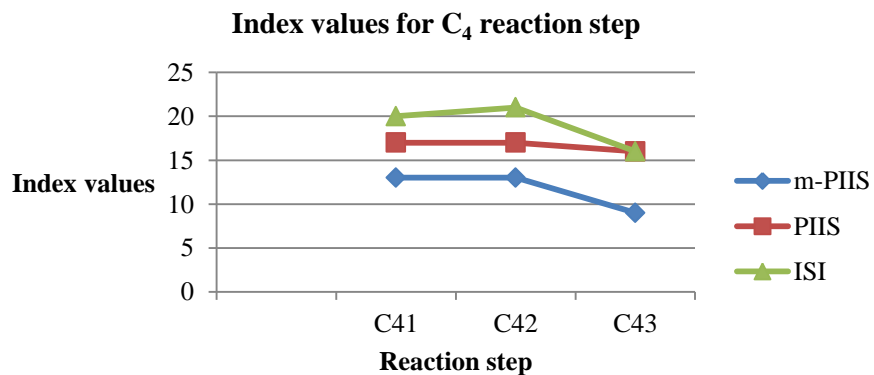


Figure 7. Comparison of index values for C<sub>4</sub> reaction steps

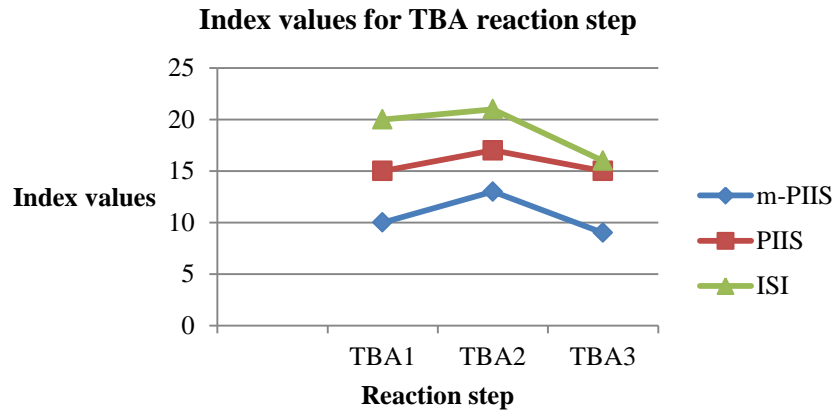


Figure 8. Comparison of index values for TBA reaction steps

Again, the new index shows a strong positive relationship with the two former indices, PIIS and ISI with a value of 0.971 and 0.817 respectively. Hence overall, the new index m-PIIS is strongly agreeable with former established indices, PIIS (r value range of 0.426 to 1.00) and ISI (r value of between 0.723 and 0.982) respectively.

#### 4.0. CONCLUSION

The developed index, m-PIIS was benchmarked against the original PIIS and ISI using the published results for the selection of process routes in MMA production. m-PIIS shows strong positive relationship with PIIS and ISI on most of the reaction step in MMA with the most significant are the C<sub>4</sub>, TBA, and C<sub>3</sub> reaction steps. Other reaction steps such as C<sub>2</sub>/MP, C<sub>2</sub>/PA and ACH do show strong positive relationship as well. This indicates that the developed index, m-PIIS is comparable to the established former indices; PIIS and ISI. Thus m-PIIS shows versatility with certain potential for future application in determining process routes selection particularly at early design stage. m-PIIS does offer simplicity and swift index computation through its features of six easily obtained and accessed parameters calculation. The index is calculated directly by summation of all assigned parameters score, via the ‘worst’ case scenario approach.

Even though m-PIIS demonstrates certain potential as an index capable of indicating and estimating the inherent safety level of a system and probably in determining the process route selection, improvements should be made to enhance its applicability. For now m-PIIS is only applicable to indicate and estimate the inherent safety level at early design stage of fuel cell system. The new index definitely has potentials to be further developed into a more concise and comprehensive index with better estimation. Introduction of other relevant and significant parameters would do more justice to this simple index. For example, the fact that fuel cell systems are electrical devices with significant hazards and the special “hydrogen-embrittlement” property are not being considered as well as inventory. The race to produce FCV with a wider range distance before refuelling does ‘force’ task player of the industry to compress more mass of gaseous hydrogen into smaller vehicles dimensions. The above mentioned factors are among the factors that should be considered if the hazards and risks of fuel cell systems need to be further understood.

For future development, m-PIIS shall be further developed and enhanced as a true representative index capable to assess and quantify the risks and hazards of the growing HFCV industry.

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