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INHERENT SAFETY INDEX FOR PROTON MEMBRANE FUEL CELL VEHICLE SYSTEM

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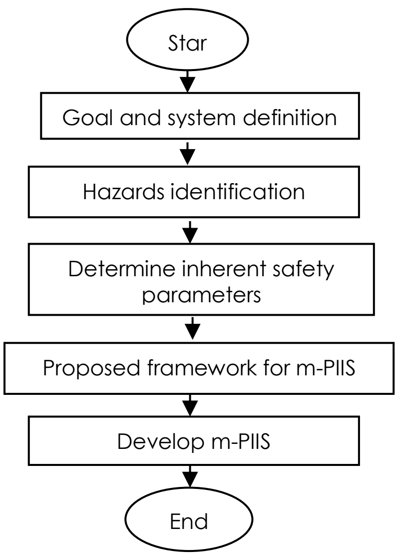
Graphical abstract



Abstract

There are enormous numbers of indices being developed in process industries to describe, rank or quantify hazards to the people, properties and environments. Most indices are being 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 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 early design stage. The developed index was applied on four proton exchange membrane (PEM) fuel cell systems; high pressure PEMFC system, low pressure PEMFC system, LH2 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 C4, TBA, and C3 reaction steps. Other reaction steps such as C2/MP, C2/PA and ACH showed a strong positive relationship as well.

Keywords: Proton Exchange Membrane (PEM) fuel cell, fuel cell system, process industry, inherent safety

Abstrak

Pelbagai indeks sedang dibangunkan dalam industri proses untuk menyatakan kedudukan atau mengukur nilai kebahayaan kepada orang ramai, harta benda dan persekitaran. Kebanyakan indeks digunakan secara skala besar dan untuk sistem proses industri yang kompleks. Pembangunan kaedah keselamatan yang pantas dan mudah dimana indeks yang wujud berkaitan dengan skala kecil, sistem membran sel bahan api kurang kompleks terutamanya satu yang akan digunakan semasa peringkat awal reka bentuk adalah penting sebagai alternatif kepada indeks semasa memakan masa yang komprehensif dan lagi. Dalam kajian ini, versi diubah suai daripada PIIS, prototaip diubahsuai indeks untuk keselamatan wujud (m-PIIS) telah dibangunkan dengan objektif mengenal pasti, menunjukkan dan menganggarkan keselamatan wujud sistem sel bahan api pada peringkat awal reka bentuk. Indeks maju telah diuji empat membran pertukaran proton (PEM) sistem sel bahan api; sistem tekanan tinggi PEMFC, tekanan rendah PEMFC sistem, LH2 PEMFC sistem dan on-board Me-OH PEMFC sistem. Indeks maju juga telah ditanda aras terhadap PIIS asal dan ISI menggunakan hasil kajian yang diterbitkan untuk pemilihan laluan proses dalam pengeluaran MMA. Keputusan telah menunjukkan bahawa m-PIIS mempunyai hubungan positif yang kukuh dengan PIIS dan ISI pada kebanyakan langkah tindak balas di MMA dengan yang paling ketara adalah C4, TBA, dan langkah-langkah tindak balas C3. Langkah tindak balas lain seperti C2/MP, C2/PA dan ACH menunjukkan hubungan positif yang kuat juga.

Kata kunci: Membran Pertukaran Proton (PEM) bahan api sel, system sek bahan api, industri proses, keselamatan yang wujud, indeks

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 the 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 as 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 the 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 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]. From 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] and as depicted in Figure 1[3].

2.1 Inherent Safety Index

In the early 1990s, several process safety evaluation methods were already existed such as Dow and Mond indices 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]. Various 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.

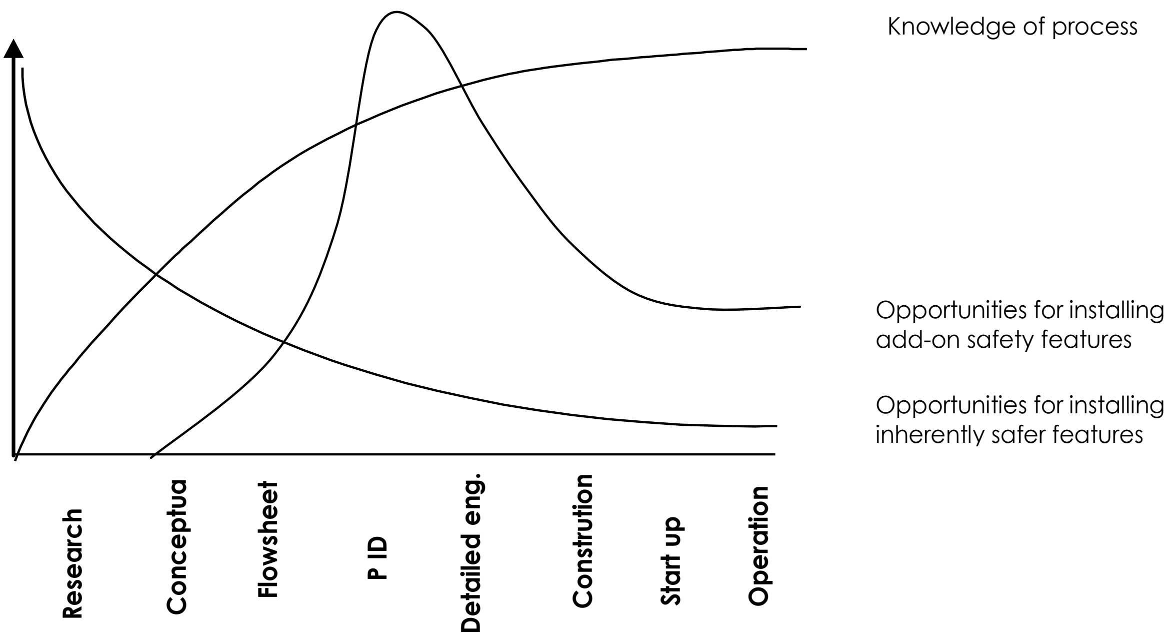


Figure 1 Design paradox and inherently safer design[3]

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.

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

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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 Figure 2.

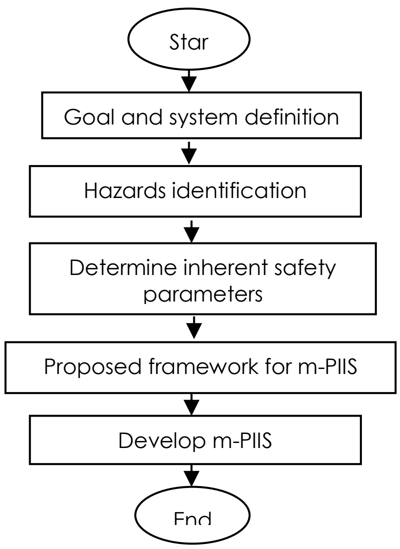

Figure 2 Steps in the development of m-PIIS

3.1 Goal and System Definition

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.

3.2 Hazard Identification of the System

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].

3.3 Determine Inherent Safety Parameters

Inherent safety parameters of the system are determined from previous literature and former indices.

3.4 Framework for m-PIIS

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].

3.5 Development of m-PIIS

Outcome of the development are further discussed in later section.

3.6 Case study

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

3.6.1 High Pressure PEMCF 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_2) 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 °C to 45 °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 to 100 km/h in 12 s.

3.6.2 Low Pressure PEMCF 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 °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.

3.6.3 LH_2 – 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_2 (LH_2 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 °C, with cryogenic LH_2 storage operating at 5 to 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 amount. This allows simple and cost efficient vehicle assembly in existing facilities.

3.6.4 On-board Methanol PEMFC System (Necar 5)

Daimler Chrysler 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 to 400 °C and 3 bar pressure. Daimler Chrysler 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_2". Daimler Chrysler 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 DISCUSSION

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 (as shown in Table 1) 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].

Table 1 Physical properties of hydrogen at 1 atm, 298K

Property	Probability / Consequence	Value
Physical state	Probability	gas
Vapour pressure (liquids only)	Probability	gas
Flammability limits (vapour only)	Probability	4 – 75 % vol. fuel in air
Flash point temperature (liquids only)	Probability	gas
Auto ignition temperature	Probability	572 °C
Ignition energy (vapour only)	Probability	0.018mJ
Heat of combustion	Consequence	285.8 kJ/mol
Max. pressure during combustion	Consequence	6.8 bar gauge
Deflagration index	Consequence	550 bar m/s

Adamson et al. (2000) [12] compare the physical properties of hydrogen and methanol in Table 2. Between hydrogen and methanol, hydrogen has the "explosive" public image and there is some 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. As described in Table 3, the 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 4, 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.

Table 2 Physical properties of H_2 and CH_3OH [13]

Property	H_2	CH_3OH
Molecular weight	2.016	32.04
Liquid density	71 (LH_2) 0.0013 (GH_2)	791
Vapour density relative to air (= 1)	14 x lighter	1.1 x heavier
Volatility (RVP – psi)	-	4.6 – 5.3
Boiling point (K)	20.27	338
Diffusion coefficients	0.61	0.0042
Explosive limits (volume %)	18.3 – 59.0	6 - 36
Fraction of heat in irradiative form	17 - 25	17
Flame temperature in air (K)	2318	-

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 [1,5,14,15,16,17,18] to demonstrate inherent safety because temperature is a direct measure of the heat energy available at release. Pressure was selected in previous literature [1,5,14,15] 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 et al. [15] ISI adopted simpler score range which is more appropriate and applicable to represent the system under investigation. Score for the most dangerous equipment was 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.

Table 3 Source of hazards in fuel cell sub-system [13]

Hazard sources	Initiating events
Sub-systems under pressure	
Fuel tank and reformer	Mechanical stress
Turbine/compressor	Overheating
Fuel cell	Vehicle accident, Corrosion (hydrogen attack)
Sub-systems in motion	
Fuel tank	Fuel loading error, Incorrect operation
Sub-systems sources of physical-induced explosions	
Fuel tank (under pressure)	Overheating
Sub-systems sources of chemical-induced explosions	
Reformer	Chemical reaction uncontrolled
Fuel cell	Electrolyte failure, corrosion
Sub-systems sources of pollution	
Fuel tank (methanol)	Corrosion
Batteries	Vehicle accident
Sub-systems sources of electric-induced hazard	Incorrect operation
Batteries	
Electrical circuit	
Systems sources of hazard related to the environment	
Environment	Bad weather

Table 4 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		√		

4.3 Development and Calculation of m-PIIS

Calculation for modified prototype index for inherent safety (m-PIIS) is based on 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.

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).

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

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.

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

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 5 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, Daimler Chrysler Necar 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 (Necar 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 Necar 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 5 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 Necar 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. Necar 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 Daimler Chrysler Necar 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 [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[17], HQI [19] and EHI [20], benchmarking step is utilising MMA process. The m-PIIS index values for each MMA reaction step are compared with the respective index values of PIIS and ISI as shown in Table 6. Figure 3 represent 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).

Table 6 Comparison of index values between m-PIIS, PIIS and ISI

Reaction step	m-PIIS	PIIS	ISI
ACH_1	17	28	25
ACH_2	12	16	21
ACH_3	10	11	21
ACH_4	10	14	19
ACH_5	14	19	19
ACH_6	10	15	18
C_2/PA_1	15	21	23
C_2/PA_2	13	26	23
C_2/PA_3	13	16	21
C_2/PA_4	11	16	16
C_2/MP_1	17	26	24
C_2/MP_2	11	10	21
C_2/MP_3	12	26	17
$C_3$1	16	24	27
$C_3$2	10	12	22
$C_3$3	10	15	18
$C_3$4	9	16	16
$C4_1$	13	17	20
$C4_2$	13	17	21
$C4_3$	9	16	16
TBA_1	10	15	20
TBA_2	13	17	21
TBA_3	9	15	16

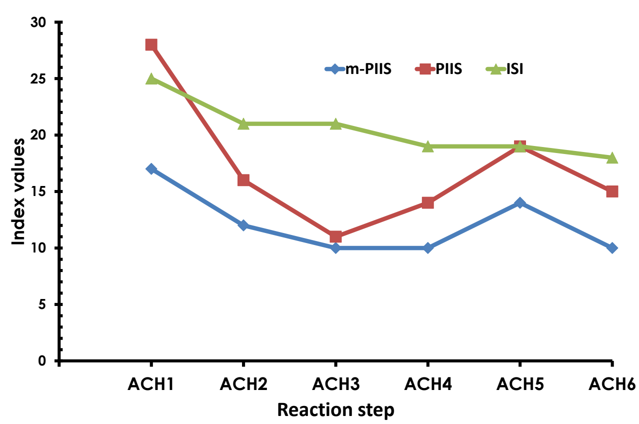

Figure 3 Comparison of index values for each ACH reaction steps

Index values for ethylene via propionaldehyde (C_2/PA) reaction steps are shown in Figure 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 ($r = 0.426$).

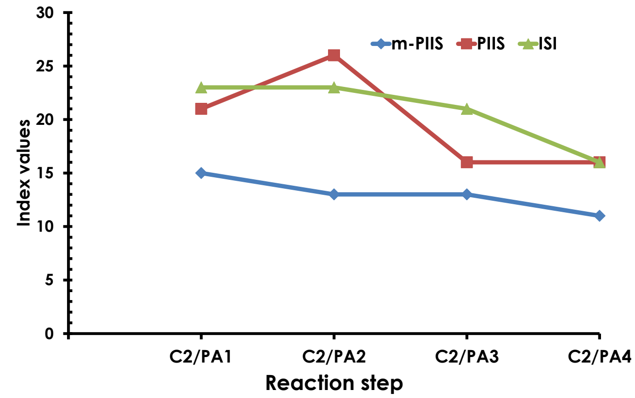

Figure 4 Comparison of index values for C_2/PA reaction steps

Figure 5 display 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 ($r = 0.629$).

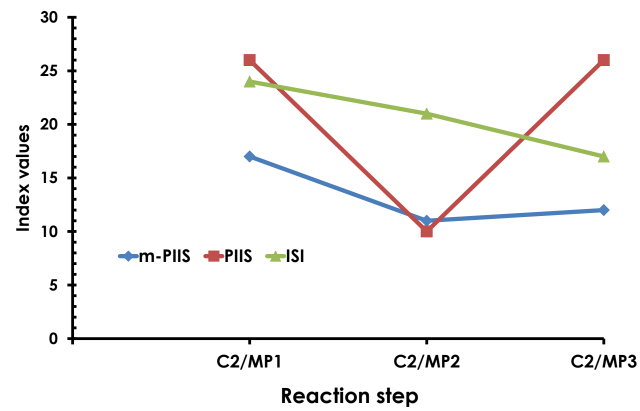

Figure 5 Comparison of index values for C_2/MP reaction steps

An index value for propylene (C_3) reaction routes is shown in Figure 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.

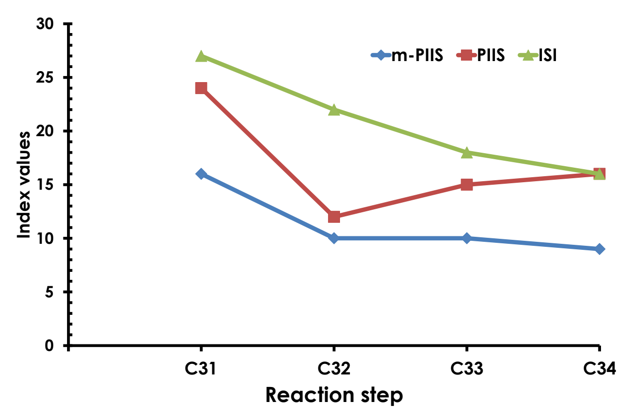

Figure 6 Comparison of index values for C_3 reaction steps

Figure 7 shows the line plots indicating the index values of isobutylene (C_4) 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_4 reaction step.

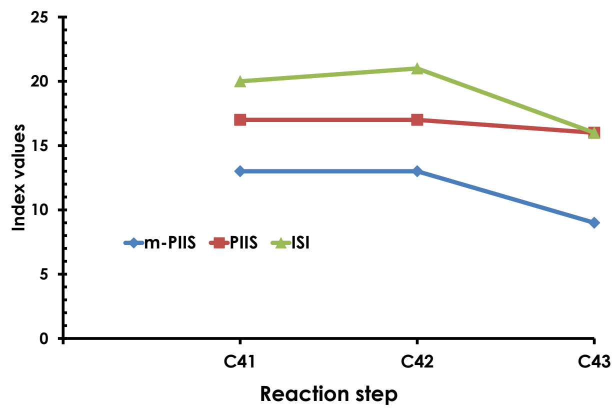

Figure 7 Comparison of index values for C_4 reaction steps

An index values for tert-butyl alcohol (TBA) process routes is describe in Figure 8. Again, the new developed 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 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.

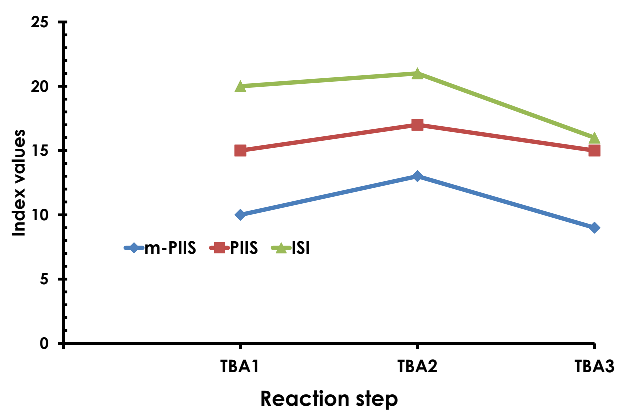

Figure 8 Comparison of index values for TBA reaction steps

5.0 CONCLUSION

As conclusion, this work has indicated that the new 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. Though, 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. For future development, it is hoped that 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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