Cost Effective Inherent Safety Index for Polymer Electrolyte Membrane Fuel Cell Systems

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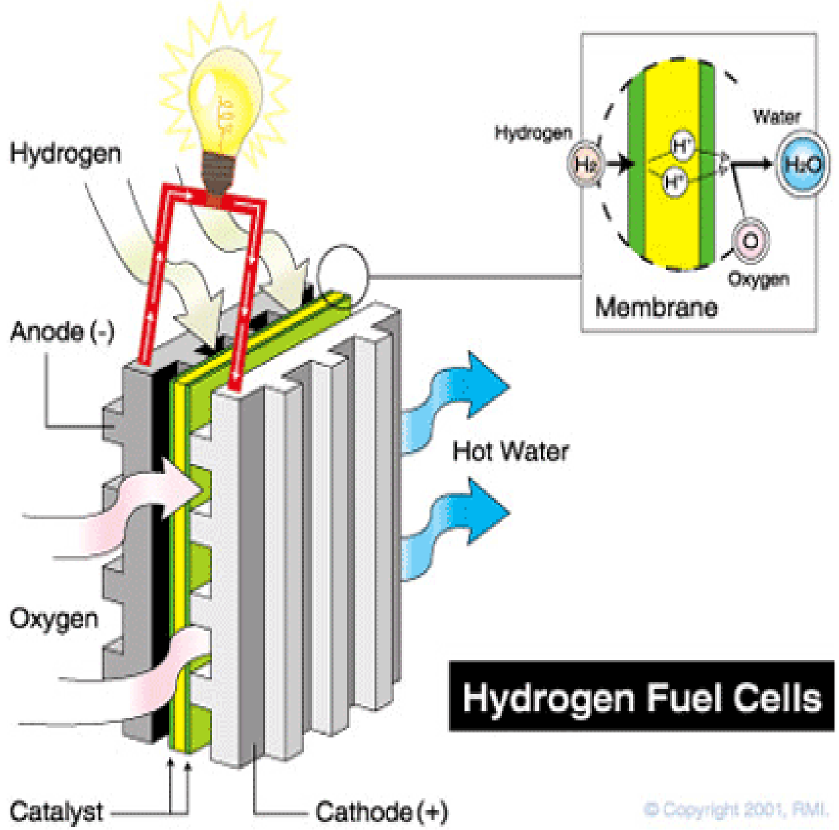
Organisation of Presentation

- Introduction
- Modified Index m-PIIS
- Case Studies
- Benchmarking of the Modified Index using MMA process route
- Discussion of Results
- Conclusion

PEM FUEL CELL



- Zero emissions – end product is just **water** & **electricity**
- High power density
- Oil independence through the use of H_2

FUEL CELL VEHICLES

GROWING NUMBERS

REPLACING Internal Combustion Engine

COMMERCIAL USE BY 2015

LOW EMISSION

RENEWABLE ENERGY SOURCES

EFFICIENT

PROBLEM - SAFETY ISSUES!!!

SAFETY INDEX

RISK

Best known measure for safety *(Heikkila, 1999*)

INDEX

single numbers / tabulation of numbers correlated to the magnitude of hazards / risk

RISK INDEX

Extensively used in process industries

Describing, ranking or quantifying hazards

Enormous numbers proposed

CURRENTLY AVAILABLE INDEX

Most Index for Large Scale Industries & Complex reactions → Dow Index, Mond Index

Existing Index - Elegant & sophisticated

(Gupta & Edwards 2003)

→ Industry prefer simpler method

(Gupta & Edwards 2002)

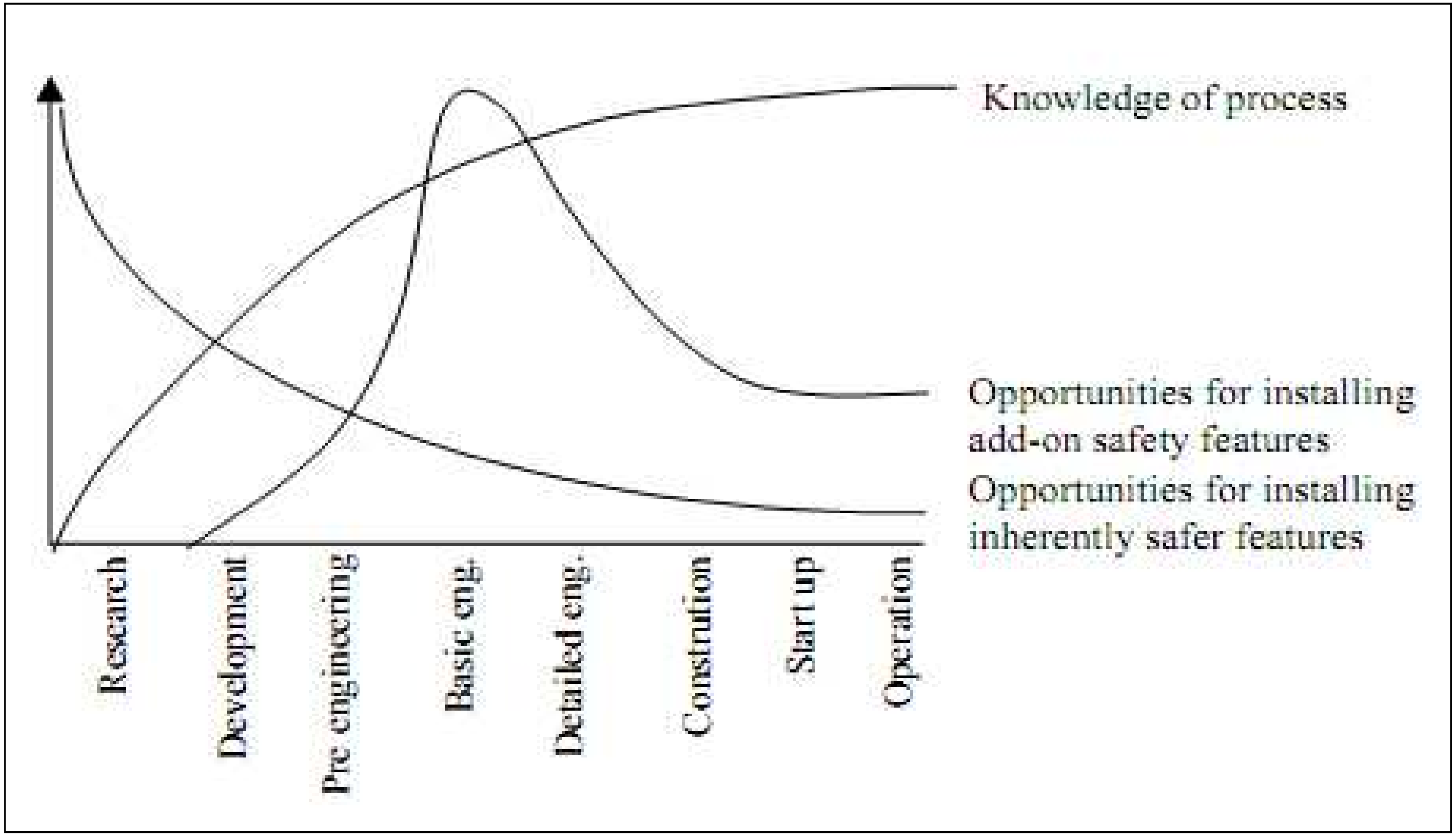
INHERENT SAFETY

Trevor Kletz (1970s)

- Intrinsic / Primary Prevention
- Common sense - avoid, minimise, substitute & simplify
- Best considered in the initial stage *(Heikkila, 1999)*
- Cost effective

DESIGN PARADOX

Figure 1: Design Paradox (Source: Hurme & Rahman, 2005)



Comparing Index

Table 1: Comparison & Selection of Parameters for m-PIIS

Inherent safety parameters	PIIS (Edwards)	ISI (Heikkela)	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		√		

PURPOSE OF THE MODIFIED INDEX

- The purpose of the modified index is to indicate & estimate the inherent hazard of Hydrogen Fuel Cell System during early design stage
- The index address the probability of hazard occurrence

The index is to act as a simple, swift & cost effective guide

The parameters selected for the index are for the **probability analysis** and not for **consequence analysis**.

Parameter of m-PIIS

- PIIS as backbone for m-PIIS because
  - it has clear advantages over other indices in early design stage
  - Normally in early design stage most of the detail process information are not available
- The index is to suit the nature of hazard of PEM which the process is simple in nature, less complex & to be applicable at early design stage (where most data are not available)

Parameter of m-PIIS

- **Five (5)** inherent safety parameters of m-PIIS are retained from the original PIIS
- **Type of equipment parameter** is taken from ISI
- **Scores** for flammability, explosiveness, temperature, and pressure and type of equipment are based on the work of *Heikkila, 1996*
- Score for **the most dangerous equipment** will be chosen as the indicator of the overall equipment safety level.
- Score for toxicity is based on the readily available **NFPA ranking.**
- Inventory & yield are omitted from PIIS because in early design stage this information are not readily available.

- Calculation of the index: **worst case scenario**
- Approach employed: **most hazardous** condition that can appear
- Low index value: an inherently **safer process**
- High index score: less safe process.

Calculation of m-PIIS

CHEMICAL INDEX:

$$K_C = F + X + T_X$$

PROCESS INDEX:

$$K_P = T + P + S_{EQ}$$

$$\mathbf{m\text{-}PIIS = K_C + K_P}$$

Flammability Score, F - Heikkila

Flammability	Scores
Non - flammable	0
Combustible (FP > 55°C)	1
Flammable (FP ≤ 55°C)	2
Easily flammable (FP < 21°C)	3
Very flammable (FP < 0°C & BP ≤ 35°C)	4
FP = Flash point BP = Boiling point	

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Explosiveness Score, X - Heikkila

Explosiveness (UEL – LEL) volume %	Score
Non explosive	0
0 – 20	1
20 – 45	2
45 – 70	3
70 – 100	4

Toxicity Score, Tx - NFPA

Classification	Description	Rating
Danger	May be fatal on short exposure. Specialized protective equipment required	4
Warning	Corrosive or toxic. Avoid skin contact or inhalation	3
Warning	May be harmful if inhaled or absorbed	2
Caution	May be irritating	1
	No unusual hazard	0

Temperature Score, T - Heikkila

Temperature (°C)	Scores
< 0	1
0 – 70	0
70 – 150	1
150 – 300	2
300.– 600	3
>600	4

Pressure Score, P - Heikkila

Pressure (bar)	Scores
0.5 – 5	0
0 – 0.5 or **5 – 25**	1
25 – 50	2
50 – 200	3
200 – 1000	4

Equipment Safety, S_{EQ} - Heikkila

Equipment items	Score, S_{EQ}
Equipment handling non-flammable, non-toxic materials	0
Heat exchangers, pumps, towers, drums	1
Air coolers, reactors, high hazard pumps	2
Compressors, high hazard reactors	3
Furnace, fired heaters	4

Case Studies

Figure 2: High Pressure PEMFC system (GM Chevrolet Equinox FCV)

Figure 4: Low Pressure PEMFC system (Hyundai Santa Fe FCV)

Figure 3: LH_2 – PEMFC system (GM HydroGen 3 FCV)

Figure 5: On-board Methanol PEMFC system (DaimlerChrysler Necar 5 FCV)

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Table 2: Summary of index values

Fuel cell system	Scores			K_C	Scores			K_P	*m*-PIIS
	F	X	T_x		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	9	3	0	3	6	**15**

- **Chemical Index (K_C)**: almost uniform, K_C is the measure of hazards contributed by **physical properties** of the fuel
- For Necar 5, **toxicity (T_X)** score is assigned 1 due to the presence of methanol
- **Process Index (K_P)**: show some variations , K_P is a measure of **operating conditions**
- Necar 5 has the highest **temperature (T)** score since it is operating at 300 - 400°C
- GM Chevrolet Equinox is assigned the highest pressure (P) score because the hydrogen gas was compressed to 700 bars

- GM HydroGen 3: **lowest index value (m-PIIS = 13)**
- DaimlerChrysler Necar 5: **(m-PIIS = 15)**
- Hyundai Santa Fe: **(m-PIIS = 15)**
- GM Chevrolet Equinox: **highest index value (m-PIIS = 16)**
- At early design stage, **GM HydroGen 3** can be considered as **inherently safest**.

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Benchmarking of m-PIIS using MMA Process Route (6 Routes)

Table 3: Correlation between m-PIIS, PIIS & ISI (using Excell)

Reaction step	Correlation m-PIIS & PIIS	Correlation m-PIIS & ISI
ACH_1		
ACH_2		
ACH_3	0.957	0.739
ACH_4		
ACH_5		
ACH_6		
C_2/PA_1		
C_2/PA_2	0.426	0.865
C_2/PA_3		
C_2/PA_4		
C_2/MP_1		
C_2/MP_2	0.629	0.723
C_2/MP_3		
C_31		
C_32	0.899	0.906
C_33		
C_34		
$C4_1$		
$C4_2$	1.000	0.982
$C4_3$		
TBA_1		
TBA_2	0.971	0.817
TBA_3		

Results & Discussion

Figure 6: Comparison of index values for each Acetone Cyanohydrins (ACH) reaction steps

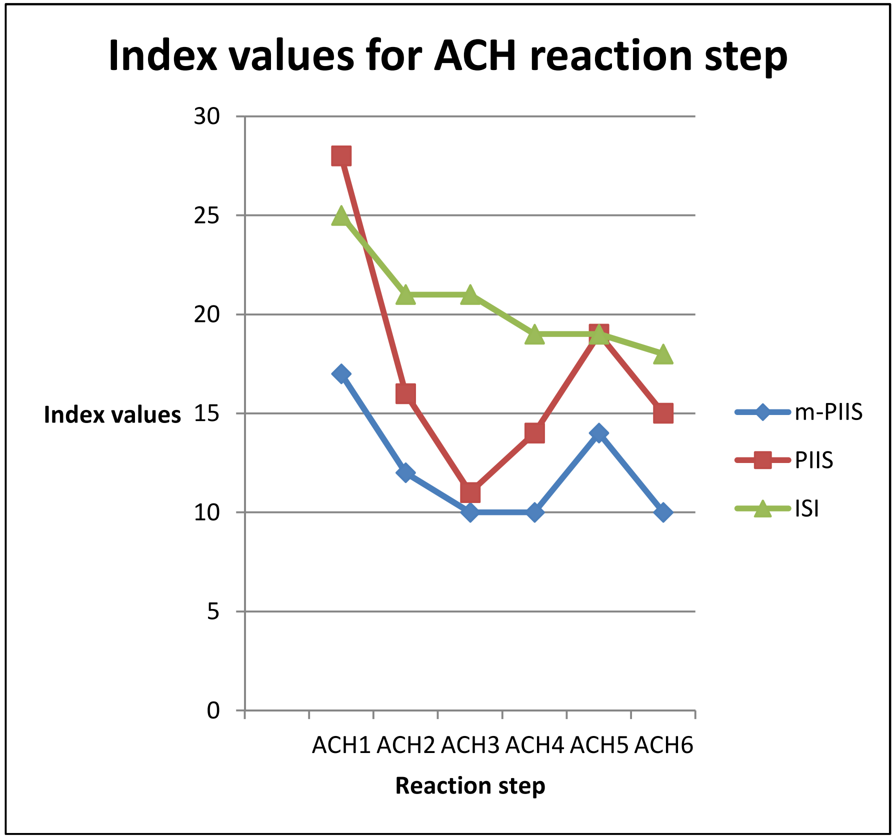
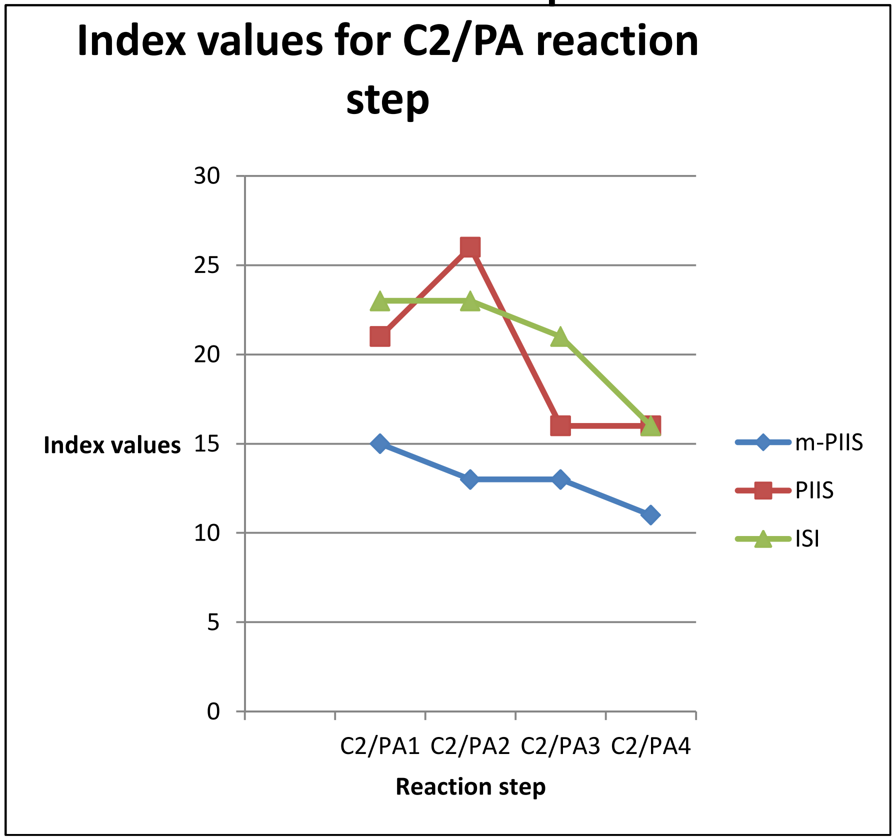


Figure 7: Comparison of index values for ethylene via propionaldehyde (C2/PA) reaction steps



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Results & Discussion

Figure 8: Comparison of index values for ethylene via methyl propionate (C2/MP) reaction steps

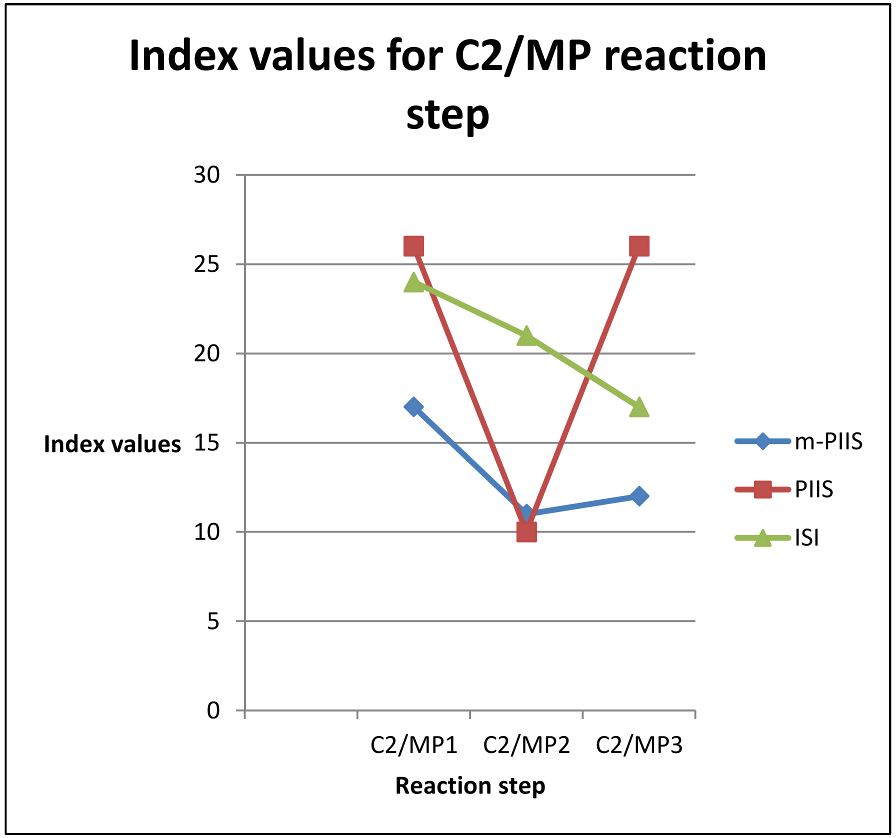
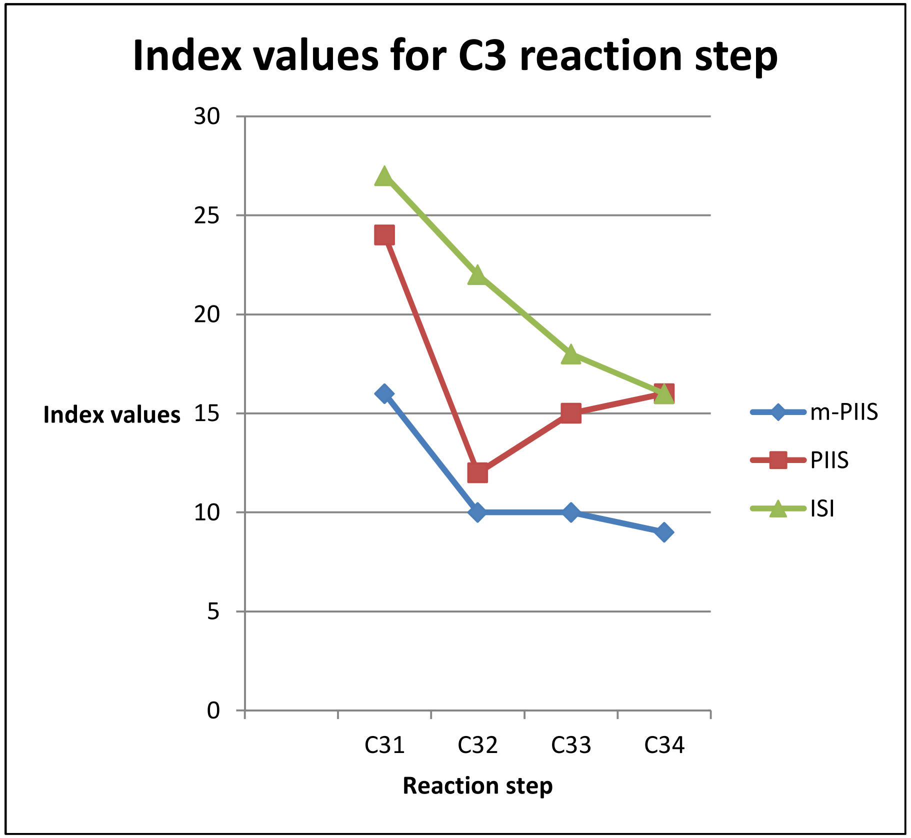


Figure 9: Comparison of index values for Propylene (C3) reaction steps



Results & Discussion

Figure 10: Comparison of index values for Isobutylene (C4) reaction step

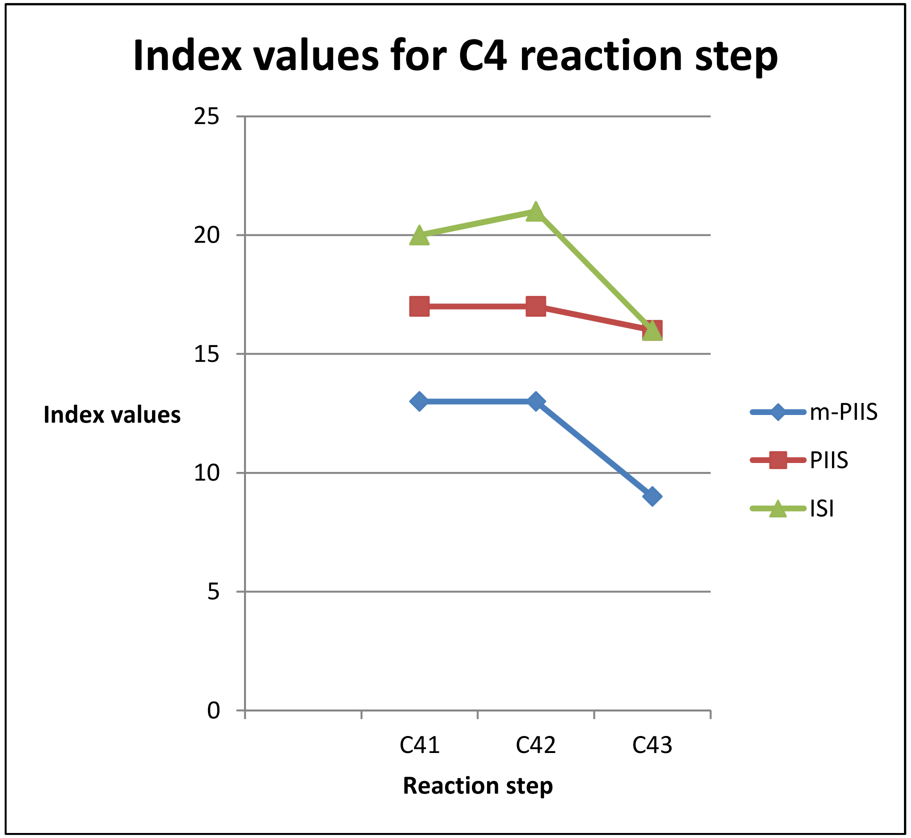
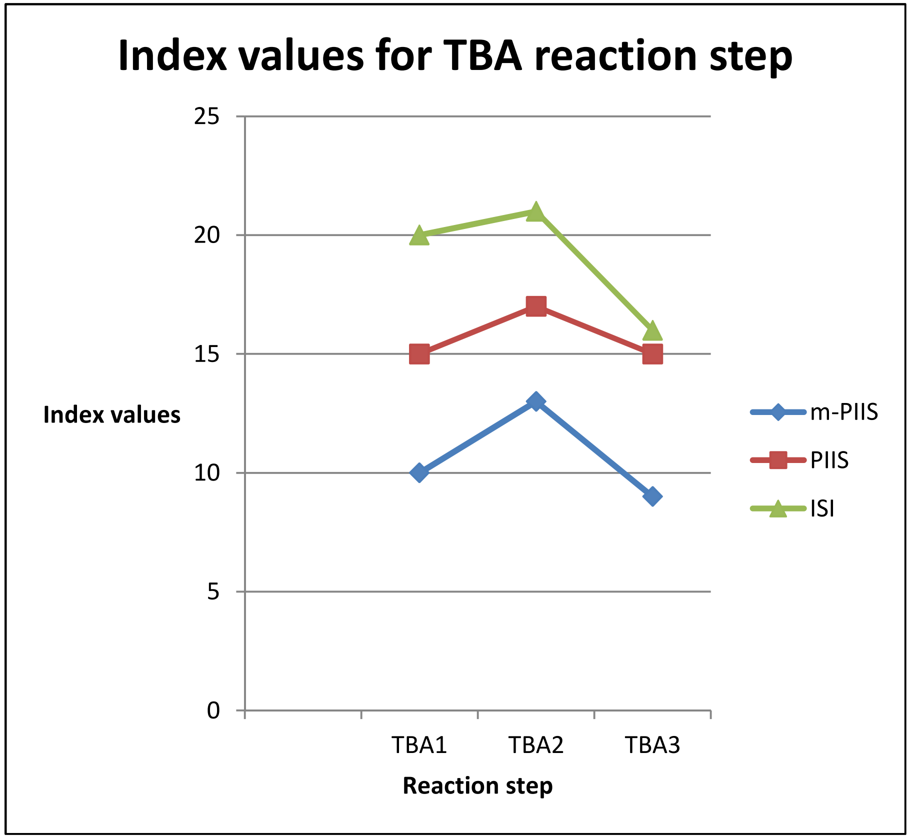


Figure 11: Comparison of index values for tert-butyl alcohol (TBA) reaction steps



Conclusion

- The modified index, **m-PIIS** is in agreement with established indices, **PIIS (r value range of 0.426 to 1.00)** and **ISI (r value of between 0.723 and 0.982)** respectively.
- It shows versatility with certain potential for future application in determining process routes selection
- m-PIIS does offer simplicity and swiftness through its features of six easily obtained and accessible parameters calculation

Recommendations

- m-PIIS has the potentials to be further developed into a more concise and comprehensive index with better estimation
- For future development, it is hope that m-PIIS shall be further refined and enhanced as a true representative index capable to assess and quantify the risks and hazards of the growing HFCV industry.

THANK YOU

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