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DEVELOPMENT OF A QUANTIFICATION TOOL FOR SOCIAL SUSTAINABILITY IN PROCESS DESIGN

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ABSTRACT: THE CONCEPT OF SUSTAINABLE DESIGN HAS EMERGED AS A NEW PARADIGM. SUSTAINABILITY COMBINES ECONOMIC, ENVIRONMENTAL AND SOCIAL ASPECTS OF PROCESS DESIGN. IN OUR RESEARCH ALL THE AVAILABLE METRICS, TOOLS THAT ARE BEING USED FOR SOCIAL QUANTIFICATION WITH GOOD DEFINITION, DESCRIPTION AND CALCULATION METHODOLOGY IS REVIEWED. THEN A NEW TOOL IS PROPOSED WHICH CONSIDERS BOTH THE INHERENT SAFETY AND OCCUPATIONAL HEALTH QUANTIFICATION FOR SUSTAINABLE PROCESS DESIGN. THE METHOD IS TAILORED FOR THE PROCESS RESEARCH AND DEVELOPMENT STAGE BY INCLUDING ONLY SUCH CHEMICAL PROPERTIES AND PROCESS OPERATING CONDITIONS WHICH ARE OBTAINABLE AT EARLY DESIGN STAGE. THE APPROACH IS DEMONSTRATED FOR THE TWO ALTERNATIVE DIMETHYL ETHER PRODUCTION PROCESSES USING SIMULATION ENGINE ASPEN PLUS[™]. WITH THE HELP OF THE DEVELOPED STANDARD INDEX SCALE AND THE RETROFITTED SUSTAINABILITY EVALUATOR THE BEST SOCIALLY SUSTAINABLE PROCESS DESIGN IS ASSESSED.

KEY WORDS: SOCIAL SUSTAINABILITY, PROCESS DESIGN, INHERENT SAFETY, OCCUPATIONAL HEALTH, ASPEN PLUS, RETROFITTED SUSTAINABILITY EVALUATOR

1. Introduction

WITH the advent of the 21st century, green chemistry is being incorporated in the design of chemical processes, eventually shifting the industrial focus from economic concerns to sustainability concerns. As economics of the industrial processes was initially dictated as the main constraint in the design of chemical process plants, health and safety of the workers and public welfare (social concerns) have only recently become another main constraint (Samli, 2011). Although researchers have put forth much efforts to quantify sustainability, an important drawback is that social quantification at the early design stage has not generally been considered from both a health and safety perspective successfully. As the term 'sense making of social sustainability' itself is abstract, a well defined methodology is needed to quantitatively measure the social dimension of sustainability.

THE proposed framework of this work incorporates the sequential process simulator, ASPEN PLUS (version 8.1) to simulate processes and calculate mass and energy balances. As part of the methodology, a modified version of the developed Excel based tool titled the "SUSTAINABILITY EVALUATOR" (Shadiya, 2010b) has been applied for addressing specifically the social dimension of sustainability.

2. Existing Evaluations Methods Discussing Social Sustainability

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MODERN process industries passed the age of add-on protective systems already and several health and safety risk assessment methods have been developed. This section describes available screening tools for evaluating various aspects of process health and safety as follows:

THE Dow Fire and Explosion Index was developed to quantify the potential damage from fire and explosion hazards in chemical processing plants that handle 1000 pounds or more of flammable, combustive and reactive toxic chemicals (Kavitha, 2003). The Dow Fire and Explosion Index have been used by many researchers to incorporate safety into chemical process design but this index system has the limitations of that it only addresses fire and explosion safety concerns but it does not address toxicological data (Shadiya, 2010a).

THE Mond Index (ICI, 1985) has been developed from the 1973 version of the Dow F&E Index. Itdiffers from the Dow fire and explosion index in that it can evaluate safety impact of wider ranges of chemicals such as explosive properties and toxicity assessments. The Mond Index also incorporates hazards credits for processes with safety control devices (Khan and Abbasi, 1998). Like Dow F&E index system, it deals only with safety concerns and not considers the long-term health effects.

NFPA 704 stands for Standard System for the Identification of the Hazards of Materials for Emergency Response which is a standard maintained by National Fire Protection Association of United States. First tentatively adopted as a guide in 1960 (NFPA No. 704M, 1969) and revised several times since then, it defines the "fire diamond" used by emergency personnel to quickly and easily identify the risks posed by materials. Although NFPA704 helps determine what, if any, special equipment should be used, procedures followed, or precautions taken during the initial stages of an emergency response it has some limitations in measuring the overall social sustainability such as the long term occupational exposure effect.

A HAZOP analysis is a procedure that is completed for existing and new facilities and it involves identifying all the hazards and operability issues in a chemical process. In the HAZOP study, the safety impact of all the different equipment found in a process, specifically looking at the potential hazards when the process deviates from design conditions is evaluated (Dunjó et al., 2010). Although HAZOP analysis has been extensively used in the chemical process industry, it has some limitations. It is time consuming, as only one accident scenario can be looked at a time. It cannot be used during conceptual stages of design, as detailed process and instrumentation diagrams must be completed, requiring knowledge and expertise in order to complete the assessment accurately (Shadiya, 2010a).

THE Hazard Identification Racking (HIRA) methodology was developed by Khan and Abbasi (1998) to evaluate the risk of fire, explosion and toxic release. One drawback of HIRA is that it does not tell if existing control systems are sufficient or need modifications. It also does not incorporate an emergency response plan such as toxic release control and firefighting equipment into the calculation (Khan et al., 2001).

EDWARDS and Lawrence (1993) have developed a Prototype Index of Inherent Safety (PIIS) for process design. The inherent safety index is intended for analyzing the choice of process route; i.e. the raw materials used and the sequence of the reaction steps. It has been argued that an overall inherent safety index, such as the PIIS, incorporates some kind of build-in judgment of the relative importance of the various types of hazards. The user has to defer to the judgment of the developer of the index or has to modify it to incorporate his own

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judgment. In the latter case the results are not any more comparable with other users (Hendershot, 1997).

THE Inherent Safety Index was proposed by Heikkila (1999) to evaluate process safety. There are two categories of safety indexes presented by this researcher and they are chemical and process safety index. The summation of these two indices yields the Inherent Safety Index. The chemical index describes how raw materials, products, by-products, and intermediates interactions affect safety of a process. While the process safety index depicts how equipment configuration and operating conditions can impact the safety of a process (Shadiya, 2010a).

IN spite of its limitation to model safety risks resulting from deviations in operation conditions, other researchers used the inherent safety index. It was integrated into an expert system called iSafe for ranking safety of process flow sheet structure (Palaniappan et al., 2002). It was used to select the safest production route from 10 different options for acetic acid (Palaniappan et al., 2004). This index was used to access the safety of simulated chemical and mechanical heat pump systems and the safest option was selected based on the inherent safety index (Ajah et al., 2008). This inherent safety methodology has been partially incorporated into the modified SUSTAINABILITY EVALUATOR for this research.

THE Dow Chemical Exposure Index CEI (1998) gives a very comprehensive method of assessing health hazards caused by acute exposure to chemicals. The assessment is carried out for each source identified to have a potential for releasing chemicals (Hassim and Hurme, 2010).

ONE drawback of CEI is that it evaluates acute health hazard risk to people based on chemical release incidents and failed to measure the long term effects on workers which is essential from occupational health point of view.

TOXICITY Hazard Index was introduced by Tyler, Doran, and Greig (1996). It ranks the relative acute toxic hazards of different chemical production units. This Mond-like index evaluates the toxicity potential of a unit, considering only short term events and acute effects based on inhalation route of exposure. It has been constructed so that the overall pattern closely follows the framework of the Mond index (Hassim and Hurme, 2010).

LIKE HIRA method (Khan and Abbasi, 1998), THI is also a safety-type assessment method which deals with acute toxicity alone and only treats the short-term accidental events, but not the low level and continuous releases.

THIS was the model developed by a working group established by the Health and Safety Commission's Advisory Committee on toxic substances (Maidment,1998; Russel, Maidmetnt, Brooke, and Topping,1998). The scheme scrutinizes both the intrinsic health hazard of substances used at work and surrogates for exposure potential particularly to employees with the ultimate target of appropriate control strategies identification.

THE shortcomings of the scheme is in its applicability for design stage implementation as it is targeted particularly for existing small and medium size plants.

THE INSET toolkit was an outcome of INSIDE Project (2001) capable of assessing SHE aspects as well as other feasibility factors. The health performance of the routes is evaluated based on the hazardous materials properties relating to health effects, the likely fugitive emission rate of that material as well as the chance that people are exposed to this. Malmen (1997) and Ellis (1997) who applied the toolkit identified some difficulties such as

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long time required in index calculation, the need to screen a large number of alternatives, and the requirement for analyzing complex issues at early stages.

THE Inherent Occupational Health Index (IOHI) was developed by Hassim and Hurme (2010) for assessing the health risks of process routes during process research and development stage by including only such properties of chemical and operating conditions of process, which are available already in this early stage. As described by Hassim and Hurme (2010), inherent occupational health strives to eliminate or reduce occupational health hazards by trying to eliminate the use of hazardous chemicals, process conditions, and operating procedures that may cause occupational hazards to the employees. The method considers both the hazard from the chemicals present and the potential exposure of workers to the chemicals. The index can be used either for determining the level of inherent occupational health hazards or comparing alternative process routes for these risks. A quantitative standard scale for the index is developed to allow health assessment of a single process. This methodology is partially incorporated in the modified SUSTAINABILITY EVALUATOR in this research.

THE Safety and Health Evaluation Tool was developed by Shadiya (2010a) as a part of her research in developing the MS Excel based SUSTAINABILITY EVALUATOR (Shadiya, 2010b) for measuring economic, environmental and social –all three dimensions of sustainability. For social quantification two categories of metrics are discussed: 1.Process Safety Risks and 2.Health Risks. Health risk assessment is adapted as disease risk assessment and incorporated in our research. A modified version of the SUSTAINABILITY EVALUATOR is also incorporated for measuring specifically the social dimension of sustainability. The modification is described in section 5.2.

ONE thing to be mentioned is that sense making of social sustainability by quantification is a complex issue. This is because it is difficult to transform social issues into scientific vision (Shadiya, 2010a). As the focus of this research is to develop new metrics and a tool for weighing of process social sustainability, besides novel metics and indices, selected metrics and indices adopted by different researchers have also been incorporated into the methodology developed.

ADVANTAGES of the framework proposed in this paper compared to other existing methods:

- 1) Although the metrics and indicators developed by other researchers were introduced in this paper, they are useful in tracking progress, not many of them are applicable to early stages of process design.
- 2) Unlike other existing methods two categories of metrics: 1) Process Inherent Safety Index and 2) Process Occupational Health Index- have been discussed simultaneously using a single tool.
- **3)** Safety indexes have been evaluated into two parts based on 1) Safety related to chemical and 2) Safety related to process- which makes the safety quantification more holistic.
- **4)** Evaluation of occupational health indexes is based on the 1) hazard from the chemicals present and 2) potential for the exposure to the chemicals which makes the comparison between the alternative processes more reliable.
- **5)** User friendly Excel based module the retrofitted SUSTAINABILITY EVALUATOR has been incorporated for social quantification which is easily amalgamable with economic and environmental sustainability for any future research.

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3. The Assessment Methodology Development

To design socially sustainable processes, the methodology shown in Figure 1 is proposed.

3.1 Simulation of the Alternative Process Designs

ACCORDING to information from the literature the base case process model is simulated. The ASPEN PLUSTM process simulator version 8.1 was used. ASPEN has phase equilibrium data available for regular chemicals, electrolytes, polymers, etc. The database is regularly updated from the National Institute of Standards and Technology (NIST). To predict phase behavior a solver is included which contains thermodynamic models. Selected process equipment and flow streams can be rigorously sized, tracked, repeated according to designers discretion. Mass and energy balance and other design calculations can be done by using built-in computational modeling tools.

3.2 Assessment of the Process Using the Retrofitted SUSTAINABILITY EVALUATOR

IN this work the SUSTAINABILITY EVALUATOR (Shadiya, 2010a) is retrofitted for evaluating only the social dimension of sustainability. The SUSTAINABILITY EVALUATOR (Shadiya, 2010b) is a novel tool that has been developed for evaluating processes for sustainability. This is a Microsoft Excel based tool which uses selected metrics and indices that address economic, environmental, health and safety concerns.

SOME of the concerns that are addressed by this tool:

- ⇒ Economic Concerns: Profit, annualized capital costs, waste treatment costs etc.
- Environmental Concerns: Atmospheric acidification, global warming, ozone depletion, photochemical smog, reaction mass efficiency etc.
- ➡ Health and Safety Impact: Health and safety risks such as risk of exposure, explosion, flammability, carcinogenic risks etc.

THE SUSTAINABILITY EVALUATOR introduces a methodology which encompasses economic, environmental and social –all three dimensions by evaluating the sustainability of a process and or compare process alternatives to select the most sustainable process.

In this research the SUSTAINABILITY EVALUATOR has been retrofitted for evaluating the social sustainability comprehensively. Specific modifications for adoption in this research are as follows:

- Social Indices as depicted from Table 1 to Table 14 are divided into two parts: 1. Total Inherent Safety Index and 2. Total Inherent Occupational Health Index. The concept of Occupational health is incorporated by the author of this paper.
- Total Inherent Safety Index has been divided into two parts. 1. Chemical Inherent Safety Index and 2. Process Inherent Safety Index. This bifurcation will help to understand the quantitative impact of safety with greater accuracy and acceptance.
- ⇒ New safety indices have been incorporated. 1. Chemical Interaction and 2. Inventory
- Equipment safety has been separately measured in inside battery limit area (ISBL) and outside battery limit area (OSBL)

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- Total Inherent Occupational Health Index has been divided into three parts. 1. Chemical and Process Hazard Index, 2. Health Hazard Index and 3. Disease Risk Index. Physical and Process Hazard Index and Health Hazard Index have been calculated based on the process reactions which is also a contribution of this research.
- Total eight different Occupational health indices have been incorporated. Six of those are from Physical and Process Hazard Index: 1. Mode of Process 2.Material phase 3.Volatility 4.Pressure 5.Corrosiveness 6.Temperature. Two of those are from Health Hazard Index: 1.Exposure Limit and 2.R-Phrase.
- ➡ For the Material Phase metric, a new criterion has been developed titled as 'continuous with recycle stream'.
- The index scale has been calibrated in this research which differs from the scale followed by different researchers so as to make a harmonious comparison between the two alternatives of DME production.

4. Case Study on Dimethyl Ether (DME) Process

THE applicability of the tool will be discussed to examine the efficacy of the retrofitted SUSTAINABILITY EVALUATOR tool and the testing of overall methodology was demonstrated using the Dimethyl Ether (DME) process case study. In this case study, there are two alternatives available for producing DME. These are via dehydration of methanol and via natural gas.

DME is an organic compound with the formula CH3OCH3. It is a colorless gas that is used as a propellant, refrigerant and as a fuel additive for diesel engines. It also acts as a precursor to produce dimethyl sulphate. Only moderate modification is needed to convert a diesel engine to burn DME. The simplicity of this short carbon chain compound leads during combustion to very low emissions of particulate matter, oxides of nitrogen and carbon monoxide. It is highly flammable but considered nontoxic. It could be used as fuel for transportation, power generation, cooking heating etc. (Ogawa et al., 2004). In China and Japan, DME is already being considered as a fuel because of the abundance of coal (Ogawa et al., 2004; Han et al., 2009).

4.1 DME Production via Dehydration of Methanol (Option 1)

IN this pathway, DME is produced by the catalytic oxidation of methanol to form DME and water as shown in Equation 5.2 below (Turton et al., 2009). The block diagram of the process is shown in Figure 3.

 $2 \text{ CH}_{3}\text{OH} \rightarrow (\text{CH}_{3})_{2}\text{O} + \text{H}_{2}\text{O}$ (5.2)

THIS process is simulated in ASPEN PLUS version 8.1. The Universal Functional Activity Coefficient (UNIFAC) is used as thermodynamic package because it predicts the properties of non-ideal mixtures well and it was recommended in literature (Jonasson et al., 1995; Kleiber, 1995).

4.2 DME Production via Dehydration of Natural Gas (Option 2)

DME production via natural gas is simulated in ASPEN PLUS version8.1, using UNIFAC, the same thermodynamic package as the previous option. The block flow diagram for this process is shown in Figure 4. In this approach, DME is produced by the following steps: steam reforming, methanol synthesis and DME synthesis in three isothermal reactors (Horstman et al., 2005). Natural gas is reacted with steam over nickel or magnesium oxide

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acting as catalysts to produce synthesis gas as shown in Equation 5.3.

 $CH4 + H_2O \rightarrow CO + 3H_2$ Methane

(5.3)

(5.4)

The reaction results in a 96.6% conversion of methane to synthesis gas. Methanol is synthesized by reacting carbon monoxide and hydrogen with the aid of carbon dioxide on alumina support as shown in Equation 5.4.

 $CO + 2H_2 \rightarrow CH_3OH$

Methanol

The reaction results in a 75.5% conversion of carbon monoxide to methanol. Lastly, the methanol is dehydrated in reactor to produce DME as shown in Equation 5.5.

 $2CH_{3}OH \rightarrow CH_{3}OCH_{3} + H_{2}O$ (5.5) Methanol DME

The reaction results in a 91% conversion of methanol to DME.

4.3 Social Sustainability Evaluation of the DME Production Processes

THE two DME base cases were simulated on ASPEN PLUS and set to a production rate of 129.70 kmol/hr and a purity of 99% (Shadiya 2010a). The two cases were quantified for social sustainability evaluation. Social impact can be categorized into total inherent occupational health impact and total inherent safety risk. The safety assessments of the two processes are compared in. As shown in the Table 16, DME via methanol has a process safety index of 52 while DME via natural gas has a safety index of 84. As depicted in Fig 5, safety risk is much less for DME from methanol than the same from natural gas.

HEALTH risk assessment was also carried out for both the chemistries of DME processes. As depicted in Table 17, the occupational health index for DME from MeOH and from NG are 26 and 222 respectively.

THE result of the disease impact assessment is depicted in Figure 6 and Table 18. As shown in the figure, for both options, the major disease risks from potential chemical exposure include developmental damage, respiratory system damage, nervous system damage and liver damage. DME production via natural gas has an additional health risk which is reproductive system damage. The chemicals resulting in this health risk are summarized in Table 18.

4.4 Selection of More Socially Sustainable DME Production Process

IN terms of social concerns, DME via methanol dehydration is more socially acceptable compared to via natural gas because the former had a lower inherent safety and inherent occupational health impact than the later. The results for safety risk evaluation as shown in Table 16, illustrates that DME production via methanol has a process safety index of 52 and is thus a safer process compared to DME production via natural gas which has a process safety index of 84. DME production via natural gas has a higher process safety index value due to the more exothermic reactions taking place in the process, more toxic chemicals, higher process temperature and the presence of compressors and high hazard reactors (Shadiya, 2010a). The results for health risk evaluation as shown in Table 17, illustrates that DME production via natural gas which has a process compared to DME production via thus a safer process compared to DME production as shown in Table 17, illustrates that DME production via natural gas which has a process compared to DME production via natural gas safety index of 26 and is thus a safer process compared to DME production via natural gas which has a process safety index of 222. The higher index value for DME production via natural gas is due to more reaction steps, high exposure

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potential for chemicals and high acute and chronic toxicity effects. As shown in Figure 6, DME production via natural gas (option 2) has a higher disease risk from the following impact categories: developmental damage, respiratory system damage, and liver damage, reproductive system damage, nervous system damage, sensory system damage compared to DME production via methanol.

CONCLUSION

IN this work a methodology was developed to evaluate to the social sustainability of processes at early design stages. In DME production study, this methodology tests the applicability of the retrofitted SUSTAINABILITY EVALUATOR with two different chemistries to assist the decision maker determines the superior socially adoptable alternative.

THE retrofitted SUSTAINABILITY EVALUATOR was used to compare two DME options that differed by reaction pathway and equipment configuration. DME can be manufactured via methanol or via natural gas. Based on the lower social sustainable impact obtained from the tool, DME production via methanol dehydration is the more sustainable production option. The lower impact value of safety and health for DME via methanol was a result of the fact that DME via methanol dehydration had a more efficient reaction process, was safer as less toxic chemicals and less hazardous equipment were present in the process and less wastes were generated in the process.

THE novel contribution of this research is that it quantifies both the inherent safety and inherent occupational health for processes at the same time based on the information available at the early design stage. Sustainability impacts for both inherent safety and inherent occupational health were incorporated into the retrofitted SUSTAINABILITY EVALUATOR. This aids the engineer in having a quantitative number to use in deciding the sustainability impact of a process for safety and health. It important to note that economic and environmental sustainability are not the direct concerns of this research but the methodology proposed here may easily amalgamable with the other two dimensions of sustainability for any future research.

WHILE this methodology would be helpful in evaluating process' social sustainability, it could be improved upon. The future research work to be considered for the future are:

- ⇒ Construct a multi-objective optimization methodology to amalgam economics, environmental with the social dimensions as objectives and their metrics as constraints.
- Figure out a more robust and effective way of entering inputs for the SUSTAINABILITY EVALUATOR from Aspen Plus e.g. linking the tool with Aspen Plus using visual basic for applications.
- \Rightarrow Validate both the health and safety impacts using other tool(s).
- \Rightarrow Develop a rigorous model for the kinetics and optimization of DME productions.
- Improve the index system by additional social metrics such as land and water impact to plant location, employee welfare, job security etc.





Fig 2: Concerns Addressed by the Retrofitted SUSTAINABILITY EVALUATOR



Figure 3: Block Diagram of DME Production via Dehydration of Methanol



Figure 4: Block Diagram of DME Production via Natural Gas



Figure 5: Results of Inherent Safety Risk Assessment from the SUSTAINABILITY EVALUATOR for the two DME Options

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Figure 6: Results of Disease Impacts Assessment from the SUSTAINABILITY EVALUATOR for the two DME Options

 Table 1: Index Score for Heat of Reaction Table

Table 2: Index Score for Chemical Interaction

Mass Enthalpy(Hf) (J/g)	Score
≤ 200	0
<600	2
< 1200	4
< 3000	6
3000	8

Chemical Interaction	Score
Heat formation	2-6
Fire	8
Formation of harmless, nonflammable gas	2
Formation of toxic gas	4-6
Formation of flammable gas	4-6
Explosion	8
Rapid Polymerization	4-6
Soluble toxic chemicals	2

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Table 3: Index Score for Flammability Index

Flammability Limits (°C)	Score
Not Flammable	0
Flash Point > 55	2
Flash Point ≤ 55	4
Flash Point < 21	6
Flash point < 0 & boiling point ≤ 35	8

 Table 4: Index Score for Explosivity Index

Explosiveness Limit	Score
Not Explosive	0
0-20	2
20-45	4
45-70	6
70-100	8

 Table 5: Index Score for Toxic Exposure Index

Toxic Exposure Limit (ppm)	Score
TLV > 10000	0
$TLV \ge 10000$	4
$TLV \le 1000$	8
$TLV \le 100$	12
$TLV \le 10$	16
$TLV \le 1$	20
$TLV \le 0.1$	24
$TLV \le 0.01$	30

Table 7: Index Score for In	ventory Index
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Inventory	Score
0-1 t	0
1-10 t	2
10-50 t	4
50-200 t	6
200-500 t	8
500-1000 t	10

 Table 9: Index Score for Pressure Index

Pressure (bar)	Score
0.5 - 5	0
0-0.5 or 5-25	2
20-25	4
50-200	6
200-1000	8

Table 6: Index Score Corrosive Index

Material of Construction	Score
Carbon Steel	0
Stainless Steel	2
Better Material Needed	4

 Table 8: Index Score for Temperature Index

Temperature (°C)	Score
< 0	2
0-70	0
70-150	2
150-300	4
300-600	6
>600	8

Table 10: Index Score for Equipment Safety Index for ISBL

Types of Equipment	Score
Equip. handling nonflammable, nontoxic materials	0
Heat exchangers, pumps, towers, drums	2
Air coolers, reactors, high hazard pumps	4
Compressors, high hazard reactors	6
Furnaces, fired heaters	8

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Table 11: Index Score for EquipmentSafety Index for OSBL

Types of Equipment	Score
Equip. handling nonflammable, nontoxic materials	0
Atmospheric storage tanks, pumps	2
Cooling towers, compressors, blowdown systems, pressurized of refrigerated storage tanks	4
Flares, boilers, furnaces	6

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Table 12: Index Score for Safe ProcessStructure Index

Process Reliability	Score
Safe	0
Sound Engineering Practice	2
No data	4
Probably Unsafe	6
Minor Accidents	8
Major Accidents	10

Table 13: Index Score for Physical and Process Hazards Index

Factor	Score Information	Score
	Continuous with recycle	2
	Continuous	4
Mode of process	Semi-continuous/semi-batch	6
_	Batch	8
	Gas	2
Material phase	Liquid	4
	Solid	6
	liquid and gas	
	Very low volatility(bp>150°C)	0
	Low(150°C≥bp>50°C)	2
	Medium(50°C≥bp>0°C)	4
	High (bp<0°C)	6
Volatility		
	Solid	
	Non-dusty solids	0
	Pellet-like, nonfriable solids	2
	Crystalline, granular solids	4
	Fine, light powders	6
	.5-5	0
	5 - 50.0	2
Pressure(bar)	50-200	4
	>200	6
	Carbon steel	0
Corrosiveness-based on construction material	Stainless steel	2

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	Better material	4
	<70	0
	70-150	2
Temperature(°C)	150-200	4
	>200	6

Table 14: Index Score for Health Hazard Index

Factor	Score Information	Score
	Vapor(ppm)	
	OEL>1000	0
	OEL≤1000	2
	OEL≤100	4
	OEL≤10	6
	OEL≤1	8
Exposure limit		
	Solid(mg/m ³)	
	OEL>10	0
	OEL≤10	2
	OEL≤1	4
	OEL≤.1	6
	OEL≤.01	8
	Acute	
	No acute toxicity effect	0
	R36.R37,R38,R67	2
	R20.R21,R22,R65	4
	R23, R24,R25, R29,R31,R41,R42,R43	6
	R26, R27,R28,R32,R34,R35	8
R-Phrase		
	Chronic	
	No chronic toxicity effect	0
	R66	2
	R33,R68/20/21/22	4
	R62,R63,R3/23/24/25,R48/20/21/22	6
	R40,R60,R61,R64,R39/26/27/28,R48/23/24/25	8
	R45,R46,R49	10

Table 15: Index Score for Carcinogenic risk

Types of Carcinogen	Group	Score
Not Carcinogenic	N/A	0
Probably not carcinogenic to humans	4	0.2
Not classifiable as to its carcinogenicity to humans	3	0.4
Possibly carcinogenic	2B	0.6

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Probably carcinogenic to humans	2A	0.8
Carcinogenic to humans	1	1

Table 16: Results of Safety Metrics from the SUSTAINABILITY EVALUATOR forthe two DME Options

Inherent safety index	Index			
, i i i i i i i i i i i i i i i i i i i	MeOH	max value	NG	max value
Heat of main reaction index	0	0%	2	25%
Heat of side reaction index	0	0%	4	50%
Chemical interaction	2	25%	8	100%
Flammability index	8	100%	8	100%
Explosiveness index	4	50%	6	75%
Toxic Exposure Index	12	40%	16	53%
Corrosiveness index	4	50%	4	50%
Temperature index	6	75%	8	100%
Pressure index	2	25%	6	75%
inventory index	4	50%	6	75%
Equipment safety index, ISBL	4	50%	6	75%
Equipment safety index,OSBL	2	25%	6	75%
Safety Level of Process Structure index	4	40%	4	40%
Total Inherent Safety index	52		84	

Table 17: Summary of Results of the Occupational Health Indexes from theSUSTAINABILITY

Health	physical an	d process	Health hazard index		Occupational health index			
index	hazard	index	Health hazard hidex				Max value	
Reaction No.	MeOH	NG	MeOH	NG	MeOH	NG	MeOH	NG
1	16	18	8	12	26	34	48%	63%
2		20		12		36		67%
3		20		10		34		63%
Total					26	222		

Table 18: Summary of Chemicals Contributing to Disease Risks for the TwoDME Options

	impact value Tonnes/yr		DME via	
Disease risk evaluation	MeOH	NG	МеОН	DME via NG
Developmental Damage	103.041	10943.034	CH3OH	CH3OH,CO
Reproductive System Damage	0	4246.69	None	СО
Respiratory System Damage	103.041	10589.303	CH3OH	CH3OH,CO,CH4,C2H6,C3H8
Liver Damage	103.041	3865.217	CH3OH	CH3OH
Nervous System Damage	103.041	4469.155	CH3OH	CH3OH,C3H8,C4H10

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