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# E-IMPACT - A ROBUST HAZARD-BASED ENVIRONMENTAL IMPACT ASSESSMENT APPROACH FOR PROCESS INDUSTRIES

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**Abstract**

This paper proposes a hazard-based environmental impact assessment approach (E-Impact), for evaluating the environmental impact during process design and retrofit stages. E-Impact replaces the normalisation step of the conventional impact assessment phase. This approach compares the impact scores for different options and assigns a relative score to each option. This eliminates the complexity of the normalisation step in the evaluation phase. The applicability of the E-Impact has been illustrated through a case study of solvent selection in an acrylic acid manufacturing plant. E-Impact is used in conjunction with Aspen-HYSYS process simulator to develop mass and heat balance data.

Keywords: Impact Assessment, Life Cycle Assessment, Normalisation, Ranking, Pollution Prevention.

## 1. Introduction

Process operation and associated activities are major sources of emissions of harmful contaminants to the environment. Environment issues are better dealt with at design stage. Therefore, it is crucial to assess the process from an environmental perspective at design as well as retrofit stages. Success of pollution prevention measures depends on the use of proper environmental assessment techniques and design tools. Life Cycle Assessment (LCA) is a useful tool for the systematic evaluation of environmental aspects of a product, service or process alternatives through all stages of its life cycle. LCA provides a means for

**Nomenclatures**

| | |
|---|---|
| $H_{tot\text{-}cat\text{-}k}$ | Total hazard to an impact category *k* |
| $H_{LCA\text{-}raw\text{-}cat\text{-}k}$ | Hazard to an impact category *k* due to the emissions over cradle-to-gate life cycle |
| $H_{pros\text{-}cat\text{-}k}$ | Hazard to an impact category *k* due to the emissions over process gate-to-gate domain |
| $H_{pros\text{-}energy\text{-}cat\text{-}k}$ | Hazard to an impact category *k* due to the emissions concerned with the production of energy consumed in a process unit |
| $H_{m\text{-}cat\text{-}k}$ | Hazard to an impact category *k* due to the emissions related to the production and supply of a raw material *m* |
| $H_{in\text{-}cat\text{-}k}$ | Hazard due to the handling of all input materials to an impact category *k* |
| $H_{out\text{-}cat\text{-}k}$ | Hazard to an impact category *k* due to all product and waste streams |
| $j$ | Number of waste streams |
| $\dot{M}_{j,s}$ | Mass flow rate of the *j* stream of the production step *s* |
| $\dot{P}_r$ | Product flow rate |
| $r$ | Number of product |
| $s$ | Number of intermediate production step |
| $Xc,j,s$ | Mass fraction of the component *c* in a stream *j* of a production step *s* |

*Greek Symbols*

| | |
|---|---|
| $\psi_{c,j,s,k}$ | Hazard to an impact category *k* due to a component c of a waste stream j in a production step s |
| $\psi_{e,k,s}$ | Hazard to an impact category *k* due to the emissions associated with the production of the energy consumed in a production step *s* |
| $\psi_{i,k}$ | Hazard for handling of an input material stream *i* to an impact category *k* |
| $\psi_{p,k}$ | Hazard to an impact category *k* due to a product stream *p* |
| $\psi_{c,j,k}$ | Hazard to an impact category *k* due to the release of a component *c* in a waste stream *j* |

environmental decision support and has been used to develop environmental friendly product and process design [1-3]. LCA consists of four phases, of which impact assessment is the most important phase due to its significant contribution to the assessment result.

For impact characterisation, two approaches are commonly used: risk based and hazard based. Risk based assessment is complicated and time consuming; however, it is more useful in critical situations. In contrast, hazard based approach is simple and less time consuming and provide qualitative environmental impact of an option. Therefore, in simple scenarios, for comparing different design or retrofit options, hazard based approach is effective.

In earlier efforts, different environmental options are compared based on an overall single impact indicator [4-5]. The indicator is the result of the summation of weighted normalized indicators of different impact categories. However, in some cases significant difference in the normalized indicators may occur among different major impact categories. This may cause the overall indicator to be biased by the impact category that has high value of normalized score [5]. Furthermore, in existing impact assessment approaches, the characterisation phase is based on one-domain life cycle inventory results and as a result the global environmental interest may override the local interest. In previous work, the authors have developed a risk-based environmental assessment approach E-Green, where all these issues are addressed [6]. In this work the authors have proposed a robust hazard-based impact assessment approach for addressing the limitations of the existing approaches. It has the following features:

i. The impact characterisation is based on the E-Green Approach [6], which proposed two-domain analysis: raw materials production and supply domain and gate-to-gate domain.

ii. Separate weighting factors are used for a particular impact category in each domain to give a different degree of emphasis to the category across the domain.

iii. The normalisation step has been replaced by a ranking step to make the decision-making process unbiased and robust.

The applicability of the E-Impact approach has been demonstrated in evaluating the environmental performance of two solvents used in an acrylic acid manufacturing process.

## 2. Description of E-Impact Methodology

The architecture of E-Impact methodology is shown in Fig. 1. The methodology is applicable at early design when designers evaluate different process options. It is equally applicable to any retrofit work of existing process systems. It consists of three steps: i) classification and characterisation, ii) ranking and iii) evaluation. The steps are briefly discussed below.

### 2.1 Classification and characterisation

In classification step, all the inventory data is classified into different classes according to their effects. For instance, classification of the emissions to air, water and soil, sorting of the air pollutants in accordance with global warming, ozone layer depletion, etc. The hazard of different emissions is calculated for each effect category. In this characterisation step, most of the earlier research has used the effect of the emissions over global, continental or regional boundary [7]. Local impact surrounding the industry is often ignored. In proposed methodology, in gate-to-gate (process) domain local impacts due to all significant industrial emissions are calculated. In order to characterize the effects of different emissions over the raw materials production and supply domain (cradle-to-gate), only criteria air pollutants and their global impacts like global warming, ozone layer depletion and acid rain are considered.

Figure 1 provides hierarchical diagram of the environmental impact. Though Fig. 1 has included most of the impact categories but it can be revised to accommodate the designers' needs.

### *2.1.1 Algorithms for hazard characterisation*

The following algorithms provide guidelines how to quantify hazard in both domains of the life cycle. The total hazard of a process option to a particular impact category k over a cradle-to-gate domain is equal to the total hazard to k category over raw materials production and supply domain plus the hazard to k category over gate-to-gate domain. This may be mathematically represented as:

$$H_{tot-cat-k} = H_{LCA-raw-cat-k} + H_{pros-cat-k} \quad (1)$$

If an energy-generating system exists outside of the process boundary i.e. energy consumed is supplied from grid, the following equation may be used to estimate the total hazard instead of equation (1):

$$H_{tot-cat-k} = H_{LCA-raw-cat-k} + H_{pros-cat-k} + H_{pros-energy-cat-k} \quad (2)$$

#### *2.1.1.1 Hazard characterisation over process raw materials production and supply domain*

To estimate hazard in this domain, one needs to consider all releases from natural resources extraction to the process gate. If $H_{m\ Cat\text{-}k}$ denotes the hazard to a category k, due to total emissions over a raw material's production and supply domain then:

$$\dot{H}_{m-cat-k} = \sum_{q=1}^{p} \psi_{t,k,q} + \sum_{s=1}^{z} \psi_{e,k,s} + \sum_{s=1}^{z} \sum_{j=1}^{n} \dot{M}_{j,s} \sum_{c=1}^{x} X_{c,j,s} \psi_{c,j,s,k} \quad (3)$$

Where, s is the number of intermediate production steps to produce the raw material (m), *j* is the number of waste streams, $\psi_{c,j,s,k}$ is the hazard of a component c to category k for a stream j of a production step *s*. $X_{c,j,s}$ is the mass fraction of the component *c* in a stream *j* of a production step s. $\dot{M}_{j,s}$ is the mass flow rate of the j stream of the production step s. $\psi_{e,k,s}$ is the hazard to category k due to the energy consumed by the process in a production step s. $\psi_{t,k,q}$ is the hazard to category k due to the energy used in a transportation step q. So, Total hazard flow rate for all the associated raw materials for a category k is:

$$\dot{H}_{LCA-raw-cat-k} = \sum_{m=1}^{n} \dot{H}_{m,cat-k} \quad (4)$$

Therefore, total hazard value for category k per unit mass of the product is:

$$H_{LCA-raw-cat-k} = \sum_{m=1}^{n} (\dot{H}_{LCA-raw-cat-k}) / \sum_{r=1}^{n} \dot{P}r \quad (5)$$

Where, $\dot{P}_r$ is product flow rate and r is the number of products.

### *2.1.1.2 Hazard characterisation over gate-to-gate domain*

In the gate-to-gate domain two types of material streams are considered: input and outgoing material streams. In addition, if energy is not generated inside the boundary of the plant then total energy consumed by the process, utility systems and other supporting systems also need to be considered to reflect the effect of energy use. If $H_{\text{in Cat-k}}$ is the hazard due to the handling of all input materials over impact category k then:

$$\dot{H}_{in-cat-k} = \sum_{i=1}^{n} \dot{M}\ \psi_{i,k} \tag{6}$$

Where, i is the number of input materials, $\dot{M}$ is the mass flow rate of an input material stream. $\psi_{i,k}$ is the hazard for handling of input material to impact category k. Therefore, for different impact categories equation (6) may be used repeatedly. The handling of input materials has a greater contribution to occupational exposure, and therefore workers health and safety. For outgoing streams, hazard is estimated using following equation:

$$\dot{H}_{out-cat-k} = \sum_{j=1}^{n} M_j \sum_{c=1}^{z} X_{c,j} \psi_{c,j,k} + \sum_{p=1}^{x} \dot{M}_p \psi_{p,k} \tag{7}$$

Where, j denotes the number of waste streams, c is the number of components in a stream j. $X_{c,j}$ is the mass fraction of the component c in a stream j. $\psi_{c,j,k}$ is the hazard to category k due to the release of component c in stream j. $\psi_{p,k}$ is the hazard for workers exposure due to handling of single or multiple products. Therefore, total hazard flow rate over the gate-to-gate domain for a particular impact category k is:

$$\dot{H}_{pros-cat-k} = \dot{H}_{in-cat-k} + \dot{H}_{out-cat-k} \tag{8}$$

The total hazard per unit mass of the product is:

$$H_{pros-cat-k} = (\dot{H}_{in-cat-k} + \dot{H}_{out-cat-k}) / \sum_{r=1}^{n} \dot{P}_r \tag{9}$$

It is important to note that unless the product life cycle is considered, the product has little impact on environmental health, however, has considerable impact on workers occupational health and safety. Therefore, in equation (7), the second term is only considered when hazard of the outgoing streams is calculated over the occupational health and safety category.

Using equations (1) and (2), one may estimate hazard over the cradle-to-gate boundary to a particular impact category. Similar procedure may be repeated for estimating hazard over other categories.

## 2.2 Ranking

In E-Impact approach, ranking has replaced the conventional normalisation step. Normalisation is usually used to compare the calculated effect scores on a common scale in order to get better understanding of the relative size of an effect. Normalisation results in a set of effect scores, which have the same or no dimension [2]. It is done using some reference values; a commonly used reference value is the average environmental load per year of an inhabitant in a specific country or region [7]. Although normalisation compares all the impact categories on a same scale, it does not say anything about the relative importance of different impact categories. Therefore, normalisation results cannot be used for final judgement. Usually normalized scores of each category are multiplied by a weighting factor, which are subsequently added to get an overall single score.

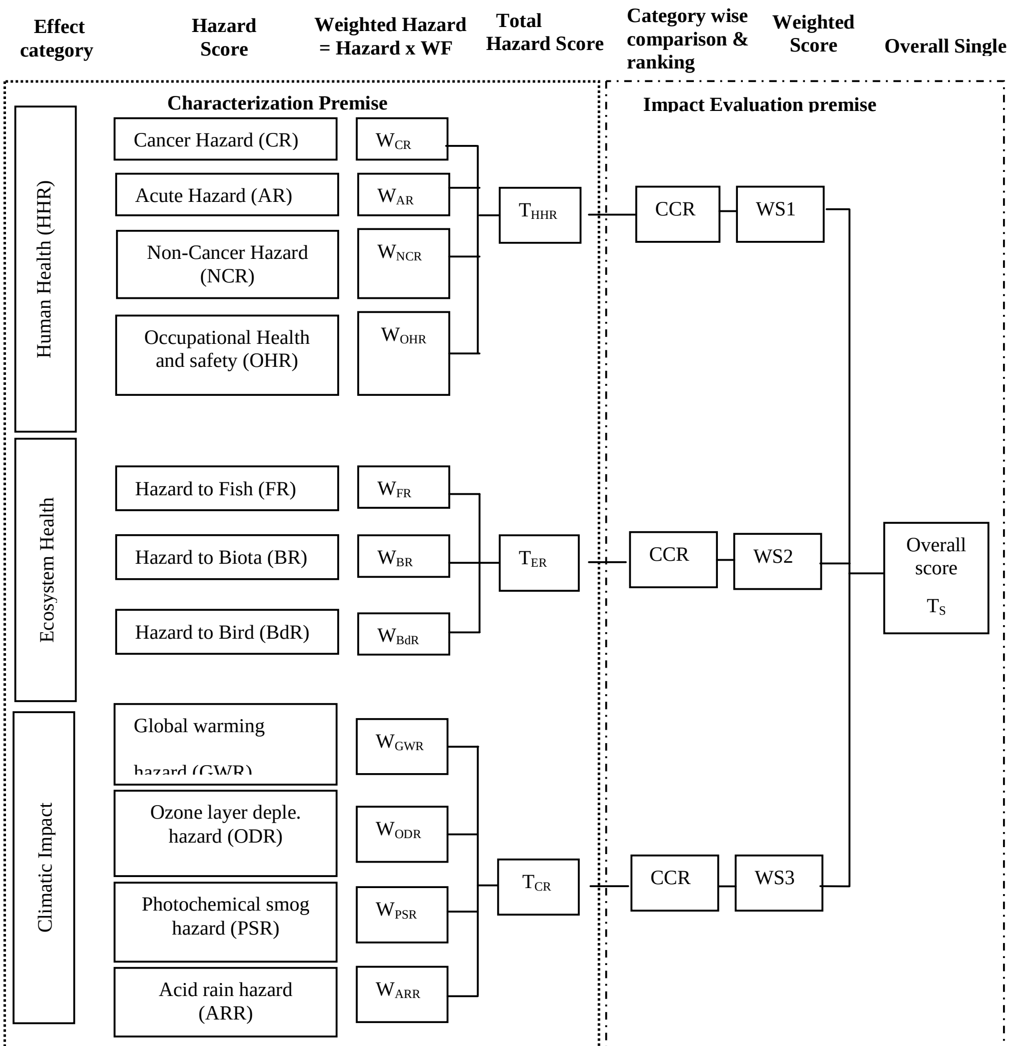


**Fig 1. Different Steps of Impact Assessment Approach (E-Impact).**

In some cases the difference among different normalized scores may be significant [5], and assigning of weighting factors may not produce reliable results as the overall single score has greater chance to be biased by the effect having higher normalized hazard score. In order to address this problem, in the proposed approach, the normalisation step is replaced by a ranking step (Fig. 1). The ranking step compares hazard scores of a specific effect category for different options and based on the comparison, different ranks are applied to the options. The hazard score of different options for a particular category k is divided by the lowest hazard score in order to assign a ranked score to each option. For instance, hazard scores for human health category of five investigated options are 70, 60, 40, 30 and 10. Therefore, calculated ranked score for the options will be 7, 6, 4, 3 and 1 respectively (Fig. 2).

### 2.3 Evaluation

Although ranking can provide a set of scores for a particular option, it cannot be used to interpret the result. Like normalisation, it does not reflect the relative importance of different impact categories. To resolve this problem ranked scores of different impact categories are multiplied by weighting factors, which are subsequently added to obtain an overall single ranked score (Fig. 1 and 2). According to the ISO 14042 [8], weighting is an optional step of life cycle impact assessment approach.

Weighting is the most controversial step of the impact assessment [2]. Weighting factors have been determined in the literature based on any of the following principles: cost of health care, pollution preventing cost, the evaluation of experts, gap between the current impact level and target level, actual damage or analytical hierarchy of the impact categories. In proposed methodology, an analytical hierarchy process is used [9-10].

Figure 2 shows process of ranking and converting the ranked scores to an overall single score using the weighting factors. Weighting factors for a specific impact category across two domains may differ, which will provide a different degree of emphasis to the impacts of each domain. If the weighting factor is same for both domains, the assessor has given the same importance to both local and global impacts.

## 3. Application of E-Impact

The applicability of the E-Impact has been illustrated in the decision-making of solvent selection in an acrylic acid manufacturing plant. The E-Impact methodology is implemented along with Aspen-HYSYS process simulator. This case has been used by the authors in demonstrating the applicability of the E-Green approach [6].

### 3.1 Process description

The process is designed to produce about 50,000 T/year of acrylic acid with purity above 99.9% [11]. Compressed air, propene and steam are fed to a reactor where acrylic acid and some acetic acid are formed through the following catalytic reactions. The reactor temperature is kept constant at 310ºC.

$$C_3H_6 + 3/2\ O_2 \longrightarrow C_3H_4O_2 + H_2O$$

$$C_3H_6 + 5/2\ O_2 \longrightarrow C_2H_4O_2 + H_2O + CO_2$$

$$C_3H_6 + 9/2\ O_2 \longrightarrow 3H_2O + 3CO_2$$

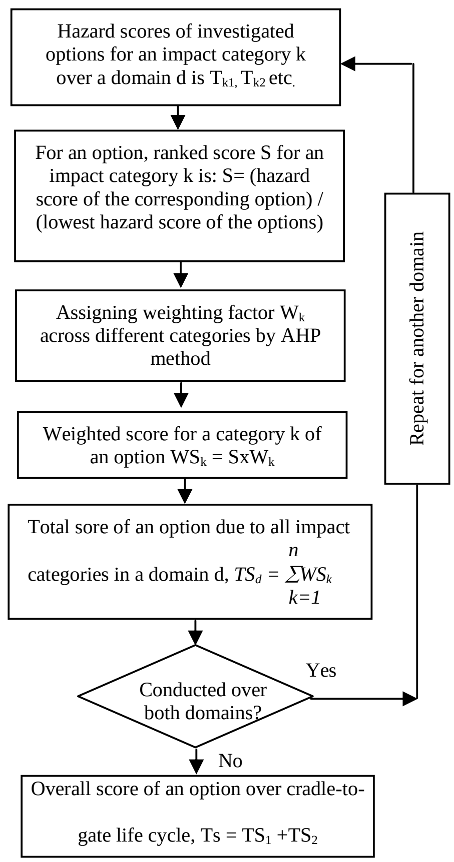


**Fig 2. Different Steps of the Proposed Ranking and Evaluation Approach**.

After the reaction, product is sent to a flash tank where it is rapidly quenched to avoid further oxidation reactions. The quenching is achieved by injecting a recycled stream of aqueous acids. The bottom product mixture from the flash chamber consists of acetic acid and acrylic acid. The vapour is sent to an absorber column where additional recovery of the liquid acid mixture is achieved. The off-gas from the absorber is released to the air.

The dilute acid stream from the absorber is mixed with the bottom acids stream of the flash tank and a portion of final stream is recycled to flash tank as quenching medium. Due to the high cost of water distillation, a solvent is used to extract the water from the aqueous acids mixture. A range of solvents could be used for water extraction, of which some common are diisopropyl ether, ethyl acetate, xylene, diisobutyl ketone, methyl isobutyl ketone and ethyl acrylate [11]. The aqueous acids are sent to an extraction column, where the acids are extracted from water using the solvent. The water is discharged as wastewater and contains trace amounts of solvent. The solvent is recovered from the acid solvent mixture in a solvent tower. The solvent is recycled back to the extraction tower. The acid mixture is sent to an acid distillation tower where acrylic acid is separated as a bottom product and acetic acid as a top product. The purity of acrylic acid and acetic acids are above 99.9% and 95% respectively.

The objective of this case study is to investigate the environmental performance of isopropyl acetate compared to a common solvent ethyl acetate. The acrylic acid manufacturing process is simulated for the both cases using Aspen-HYSYS process simulator.

### 3.2 Inventory analyses and impact assessment

Table 1 shows the input materials and waste flows of the acrylic acid plant for the two options. In waste stream only trace components are shown. For life cycle inventory analysis of raw materials, all the intermediate production steps starting from the natural sources are considered. To calculate the environmental burdens, energy consumed in process and transportation, and important hazardous releases in each production step are taken into account. The significant emissions of the two solvents over each domain due to energy used, manufacturing and other activities are shown in Table 2, which are calculated with the help of ecoinvent life cycle database [12].

For estimating hazard of a chemical for a particular category, hazard index from RSEI database has been used to obtain the potential hazard of a chemical per unit mass [13]. Then the Equations (1-9) are used to quantify the hazard over the investigated domains. The overall score for a particular option over the investigated life cycle domain is calculated using the proposed impact assessment method (E-Impact).

## 4. Results and Discussion

Figure 3 presents the ranked score of the two solvent options for human health category over the gate-to-gate life cycle domain. It is shown that the isopropyl acetate option has lower score compared to the ethyl acetate option, which indicates that the isopropyl option is superior in human health impacts. In Fig. 4 the comparison of the two options in gate-to-gate domain in terms of ecological impact is shown. From Fig. 4 it is distinct that the isopropyl acetate option has less impact on ecological health compared to the ethyl acetate option due to its lower score. The climatic effect for the two investigated options over the gate-to-gate (local) domain is presented in Fig. 5. It shows that the both options have equal climatic impact score. This is due to the fact that production rate and composition of the off-gas remains same for the both options (see Table 1) and the effect of energy on climate consumed within the process boundary is not considered over the gate-to-gate domain.

**Table 1. Flow Rate of Input and Waste Streams of Acrylic Acid Plant.**

| | **Ethyl Acetate Option** (Base case) | **IsoP-Acetate Option** (Alternative case) |
|---|---|---|
| **Input materials** kg/h | | |
| Propylene | 5,400 | 5,400 |
| Steam | 18,000 | 18,000 |
| Air | 39,000 | 39,000 |
| Ethyl acetate | 44,053 | |
| Isopropyl acetate | | 61,280 |
| **Off-gas composition,** kg/hr (mass flow) | | |
| Propene | 730.8 | 730.8 |
| $CO_2$ | 2607.2 | 2607.2 |
| ***Waste water composition*** | | |
| **Mass flow, kg/hr** | | |
| *Ethyl acetate* | 2013.2 | 558.3 |
| *Isopropyl acetate* | 13.6 | 2.22 |
| Acetic acid | | |

Figure 6 compares the climatic impact of two options over the raw materials production and supply domain. It is observed that the isopropyl acetate option has higher value of ranked score in this domain, which indicates that the amount of total toxic contaminants released in the isopropyl acetate production and supply domain has higher overall hazard to climate compared to that of the ethyl acetate option. From Figs. 3-6, it is distinct that one option does not always result in better environmental performance as compared to the other option for all impact categories over both domains. The importance of different impact categories is not same for a particular domain and it might also vary across the domain. Therefore, the option, which has a lower ranked score over more impact categories, is not necessarily the preferred option. It is very difficult for the analyst to take decision in this complex situation. The situation will increase complexity as the number of options increases. To overcome this issue, all the ranked scores for a specific option over the cradle-to-gate domain are converted to an overall score by using weighting steps (Figs. 1 and 2). Figure 7 presents the overall ranked score of the two options over their cradle-to-gate life cycle domain. Figure 7 shows that the isopropyl acetate option has lower overall ranked score than the ethyl acetate option, which indicates that the isopropyl acetate option is overall more environmentally friendly considering both global and local impacts. In Figure 7, the hazard-based approach shows that the isopropyl acetate option is about two times better than the ethyl acetate option. However, the corresponding risk-based result (Fig. 8) shows that isopropyl acetate option is about five times better. The difference in results between the two effect characterisation approaches are due to the fact that hazard does not consider the site-specific parameters, therefore, significant changes occur during multi-media fate and transport of the chemicals.

**Table 2. Contaminants Emissions Data for the Two Solvents over Investigated Domains** (for 1 kg solvent).

| **Contaminants** | **Ethyl Acetate Option** | | **Iso P-Acetate Option** | |
|---|---|---|---|---|
| | Gate-to-gate domain Kg | Raw material domain Kg | Gate-to-gate domain Kg | Raw material domain Kg |
| $CO_2$ | 0.062 | 1.568 | 0.049 | 1.651 |
| CO | - | 0.005 | - | 0.004 |
| $SO_2$ | - | 0.006 | - | 0.006 |
| $NO_x$ | - | 0.005 | - | 0.005 |

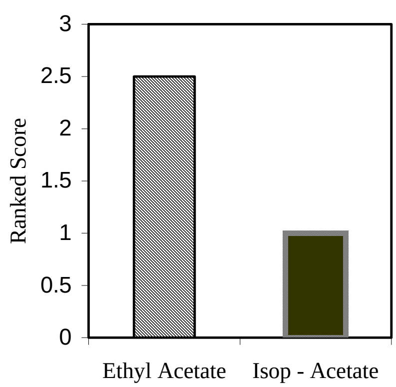


**Fig. 3. Human Health Ranked Score Obtained for Both Options Over Gate-to-Gate Domain.**

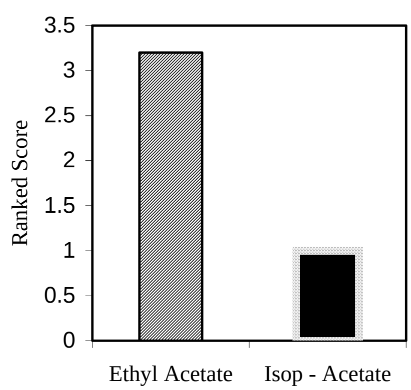


**Fig 4. Ecological Health Ranked Score Obtained for Both Options Over Gate-to-gate Domain**.

## 5. Conclusions

In this paper an impact assessment methodology (E-Impact) for process design and retrofitting is presented. It has significantly modified the conventional impact assessment approach. It has following features:

i. In characterisation phase, the effects are characterized based on two domains; inventory analysis: raw materials production and supply domain, and gate-to-gate domain, which helps to characterize and evaluate the impacts separately in two domains according to the needs. It would help to select the option, which is benign from both global as well as local environmental perspectives.

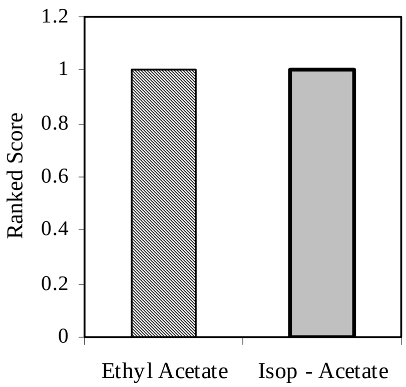


**Fig 5. Climatic Impact Ranked Score Obtained for Both Options Over Gate-to-gate Domain.**

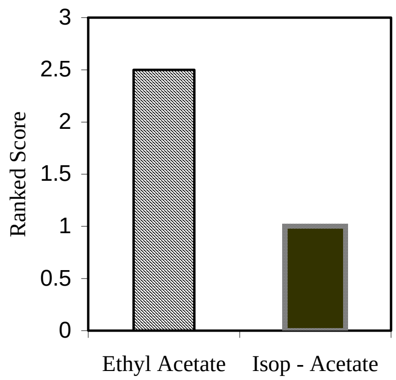


**Fig 6. Climatic Impact Ranked Score Obtained for Both Options Over Raw Materials Life Cycle Domain.**

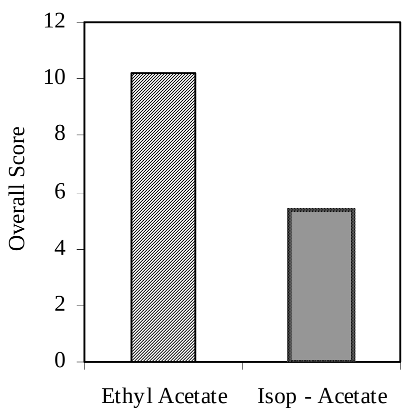


**Fig 7. Overall Score Obtained for Both the Options over Cradle-to-gate Domain.**

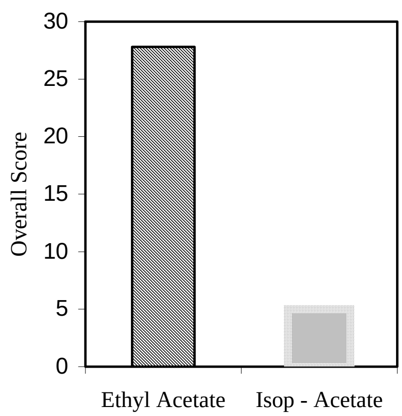


**Fig. 8. Overall Score Obtained by Risk Based Approach for Both Options over Cradle-to-gate Domain.**

ii. It has replaced the conventional way of normalisation by a ranking method. This attempt has been made to completely eliminate the potential biasing effect on the overall single score caused by the significant difference of the normalized scores across the impact categories. The ranking is much easier and less time consuming, which would make the E-Impact a robust environmental impact assessment tool for process industries.

The ranking approach is equally applicable for the cradle-to-grave LCA for assessing products or services. From the case study, it has been realized that E-Impact approach is easily applicable and less time consuming. A significant difference is observed between the results obtained in hazard based and risk based impact characterisation. Therefore, for critical decision-making risk-based effect characterisation approach should be adopted. E-Impact is still at early stage of its application, however, research is continuing to apply the E-Impact in different real life case studies to check its robustness in diverse process scenarios.

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