**SUSTAINABILITY FOOTPRINT METHOD FOR DECISION MAKING**

**Introduction**

Unambiguous decisions on system performance, when the indicator datasets constitute numerical values of many indicators, are not easy to make. The choice of the set of indicators is determined a priori; in other words, the indicators are constructed first, followed by data collection and computation of these indicators. In most of the current practices, little or no analysis is performed for the indicators after the calculation of the values, but emphasis is given to tracking the values of the indicators themselves. To represent the indicators, a radar chart or star plot is used in most cases, and a unique decision point is never reached for overall performance of an option within the system. The radar plot, a visual diagram, can handle only a few indicators and fails when the system is defined by a large number of indicators. Also, because the data gathering and processing steps involved in the indicator calculation are resource-intensive, there is a significant need to identify whether an indicator is truly necessary for ascertaining the sustainability of a system. In other cases, where such data aggregation and representation is reported by a handful of companies, the underlying methods are not disclosed. A transparent and quantitative numerical aggregation method for one sustainability index for decision making is needed, and we are presenting that discussion next.

**Rationale: Need for Decision Making using Metrics and Indicators for Sustainable Manufacturing**

No effort has been proposed by the AIChE or the IChemE to combine any indicator information into a single index. This makes it a data collection process without significant analysis on assessing the path towards sustainability. However, with such high quality numerical data using the indicators, significant progress can be made by identifying potential process improvements, the environmental impacts of the products and processes, or the health and safety improvements that have been achieved in a company, with respect to itself, and also with respect to other companies that report data within a similar scope. With further availability of temporal data these process metrics can be used to track sustainability performance over several years. BASF’s methods of eco-efficiency analysis or SEEBALANCE® methods do not suffer from this problem because they express the measures of the three pillars of sustainability in composite forms, thus allowing an easy visual inspection for a decision. However, as we pointed out before, the methods of aggregation for creating the composite indices, especially representing environmental and societal impacts are not publicly known. Hence we present a method that is efficient in making decisions regarding sustainability performance of processes based on indicator data.

**Course Content: Background on Aggregate Index, Steps in the Sustainability Footprint Method**

***Background on Aggregate Index***

The radar plot constitutes an n-dimensional polygon where n is the number of indicators. When several alternative options are represented on such a diagram, an easy decision is hard to make from the clutter of the data, especially when the number of indicators is very high. For this reason, various authors have argued in favor of a single aggregate sustainability index derived from these indicators (Hák et al., 2007, Nardo et al., 2005). The aggregate sustainability index is a numerical composite of underlying indicators that reflects, in aggregate, the state of the system in question as measured by the values of the individual indicators. Aggregate indices are distinguished from composite indices where composite indices are composed of more fundamental indicators, and not necessarily a numerically related sum. Seminal work has been done in this direction for composite index as captured in the Fisher Information (Cabezas and Fath, 2002, Fath et al., 2003). Fisher information has been successfully applied to ecological systems to study regime shifts and resilience of systems. However, in their methodology, Fisher Information is used as one indicator along with other indicators for sustainability assessment. Although the methodology of Cabezas et al. has been applied before for regional systems (Type II), it is being applied now to product systems as well (Type IV) (Ingwersen et al., 2014).

Aggregate indices, on the contrary, are numerically combined indices of individual indicators which can be used to rank technology or policy options for a system. Decision-making with integrated information on sustainable development of a company has been demonstrated using the composite sustainable development index (ICSD) in order to track data on economic, environmental, and social performance of a company with time (Krajnc and Glavič, 2005). For countries, aggregate indices have been used to compare their competitiveness, innovative abilities, degree of globalization and environmental sustainability (Freudenberg, 2003).

For engineering applications, aggregate indices have not been widely used to assess the overall sustainability from environmental, economic and social indicators. Some efforts which are currently being pursued tend to look at sustainability from different perspectives. For example, the Sustainable Process Index (SPI) is based on the assumption that sustainable flow of solar exergy is required for a sustainable economy (Narodoslawsky, 2015). The conversion of the solar exergy to services needs area which then becomes the limiting factor of a sustainable economy. A measure of areas added over the life cycle of a product gives the indicator of interest. The AIChE/CWRT Total Cost Assessment Methodology (TCA) (Beaver, 2000) effort calculates the overall sustainability by assigning an economic value to various aspects of sustainability, and aggregating them to a single dollar amount shows another method of aggregation. Sengupta and Pike (2012) demonstrated the use of the TCA method by maximizing a triple bottomline profit for determining the sustainability of an industrial complex, and quantified economic, environmental and societal aspects into a single value measure for optimization. This methodology is useful when reliable costs are available for the three dimensions of sustainability assessment. Singh et al. (2007) also developed a sustainable performance for comparing steel industries. They have used hierarchy process (AHP) to calculate weighting factors of the indicators. The use of the composite sustainable development index (ICSD) has been used to study the sustainability assessment of breweries (Tokos et al., 2012). Brandi et al. (2014) has used Canberra metrics to aggregate sustainability metrics and have shown the application of their method in different chemical processes. Olinto (2014) has used vector space method for aggregating sustainability indices and shown the results for different industrial processes. Thus, aggregate indices are useful for their ability to integrate large amounts of information into easily understood formats. However, one needs to be careful in the construction of aggregates as methodological difficulties often hinder the implementation of these indices.

The use of an aggregate index may trigger the curiosity to know how each indicator has contributed towards the aggregate indicator. This is helpful particularly when a large number of indicators are integrated and meaningful inferences are sought. A sustainability footprint De or D (respectively called Euclidean Distance and Geometric Mean distance) can be constructed by measuring a statistical distance between a multidimensional system and another similar and relevant multidimensional reference system. Given that the value of the sustainability footprint is available, the contribution of the indicators in the entire dataset of system options is analyzed using a multivariate statistical analysis method known as partial least squares-variable importance in projection method (PLS-VIP). Thus, the aggregate index helps to rank the options in the system, and the PLS-VIP method is used to rank the indicators in the system. Together, they complete an analysis and reinforce decisions taken with respect to relative sustainability of a system.

***Steps in Sustainability Footprint Analysis using the AI-PLS-VIP method***

The steps in constructing composite indicators are discussed in the following sections.

*Step 1: Ensure Quality and Unidirectionality of Indicator Data*

The first step in any indicator-based analysis starts with ensuring availability of good quality data. Step 1 of the AI-PLS-VIP method starts after data have been collected for the system options using indicators that credibly characterize the particular system. It is absolutely necessary to have indicator data for all the system options. If some indicator data are missing for one of the options, then the following actions may be used to determine the missing information (Freudenberg, 2003).

* *Data deletion*: omitting entire records (for indicators or system options) when substantial data are missing. Deleting data entirely for an option takes that option out of consideration, however.
* *Mean substitution*: This method takes the average of the remaining values of the same indicator, thus substituting a mean value computed from the other options available to fill in missing values. This can be used for temporal data.
* *Regression*: using regressions based on other indicators to estimate the missing values. This is useful when temporal data on indicators are missing for a certain option.
* *Nearest neighbor*: identifying and substituting the most similar case for the one with a missing value.
* *Ignore value*: This is essentially assuming a numerical value of zero for the indicator. Care must be taken here to confirm that ignoring the value is physically consistent, i.e. the indicator is actually zero. Otherwise some of the other methods above should be applied.

For making sustainability inferences, a system option having a smaller aggregate value of the sustainability footprint is considered more sustainable, in accordance with the convention that each indicator is fashioned in a way in which lower numerical values are more desirable than higher ones. To ensure this, an effective method for making all the indicators unidirectional is necessary. This can be done in two ways. The first method is to design an indicator with attributes that make lower values better and higher values worse. The second method is to transform an existing indicator to make it conform to this convention. For instance, if an indicator value is given as a percentage and higher percentage means better performance, then the indicator is changed by subtracting the value from 100. If an indicator value is not given in percentage, it can be transformed into a new indicator where an inverse of the original value can be used for complying with the convention. Thus, indicator data quality and unidirectionality are the prerequisites for assessing sustainability using the AI-PLS-VIP method.

*Step 2: Compare Relative Sustainability of Options: The Aggregate Index Method for Sustainability Footprint*

The second step in the AI-PLS-VIP method is the creation of the aggregate index for calculation of the sustainability footprint. Aggregate indices have been studied in the past for determining sustainability of systems. For example, the aggregate index, *D*, proposed by Sikdar, 2009 can successfully compare competing processes or products. However, *D* had limitations in the method when the indicator values could have a negative or zero numerical value such that the ratio will be negative. To overcome this, the *De* process is proposed (Sikdar et al., 2012). Later however this difficulty of *D* was overcome by synthesizing a reference point. Currently both sustainability indices conform to the AI-PLS-VIP method.

The aggregate index computation involves two parts. The first part is the normalization of the indicators and the second part is the computation of the aggregate index.

Several techniques can be used to standardize or normalize the indicators. This step is important because the indicators characterizing a system are various, with different scales and units of measurement. Commonly used methods of normalization (Freudenberg, 2003) depending on the system being studied include the following:

* *Standard deviation from the mean*, which imposes a standard normal distribution (*i.e.* a mean of 0 and a standard deviation of 1) on the data. Thus, positive (or negative) values for a given system option indicate above (or below) average performance: 
* *Distance from the group leader*, which assigns 100to the leading option and other options are ranked as percentage points away from the leader: 
* *Distance from the mean*, where the (weighted or unweighted) mean value is given 100 and data receive scores depending on their distance from the mean. Values higher than 100 indicate above-average performance: 
* *Distance from the best and worst performers*, where positioning is in relation to the maximum and minimum in the data set and the index takes values between 0 and 100: 
* *Categorical scale,* where each variable is assigned a score (either numerical such as between [1…k], k>1, or qualitative - high, medium, low) depending on whether its value is above or below a given threshold.

For the AI-PLS-VIP method, we used the distance from the best and worst performers by adopting a synthetically chosen point in this space represented by the minimum values of the indicators encountered in the system. These indicators will represent an ideal case of a synthetic reference option *X0*.Thus, with respect to *X0*, any of the real options will always have positive difference of the indicator values. This is essentially shifting the point of reference from one of the options to an imaginary option, and the exercise is to find out how far a real option is from the reference option. In addition, if the indicator values are defined such that higher values are worse than smaller values, then a smaller difference of an option from the imaginary point would be more sustainable than one with a larger difference.

After normalization with respect to the *X0*, the calculation of the aggregate index is computed by using the Euclidean distance method as shown in Equation 1.

 (1)

where *De,m* the measure of relative sustainability,is the Euclidean distance of a chosen option *m* having indicators *Xj*, at a point in time obtained after normalizing with respect to a synthetic reference option *X0*. The idea of the arbitrary reference option in *De* calculation is to transform the dataset to avoid occurrence of negative data points in the transformed data. The weighting factor *cj* allows use of weighting preference (usually a societal choice) of any of the indicators in comparison to others. While considering time series data for options, the datasets can be represented by a *m×n×t* matrix, where *m* is the number of options, *n* is the number of indicators, and *t* is the number of temporal points. A *De* value is computed for each system option each year.

Another method to compute the aggregate index is to use the geometric mean from a carefully normalized set of indicators. This normalization is achieved by a similar shifting of the reference point to ensure positive non-zero values (Sikdar et al., 2012). Equation 2 represents the geometric mean of the ratios of the indicator values when any option is compared with only the reference option constituted with the minimum values assumed by the indicators for that data set. In this case, the ratio of the lengths of the indicators from a fixed minimum is considered for the geometric mean approach.

 (2)

where *xi*0 is the minimum value assumed by the indicator *i* in the dataset and constitutes elements of the vector, ***X****0*. The distance will be zero where *xi*=*xi*0, hence an offset from the minimum value is required for Equation 2 to work. We can offset the point of reference arbitrarily with a constant, C*offset*, so as to have all indicator distances greater than zero. Sikdar et al. 2012 discusses the selection criteria and effect of C*offset* on the value of *D*.

Both *D* and *De*can be used to calculate the aggregate index in comparing the relative sustainability of options. We have used *De*in this chapter for demonstrating the applicability towards assessing sustainability of systems.

### Step 3: Compare the Ranking of Indicators: Partial Least Square-Variable Importance in Projection Method

The third step in the AI-PLS-VIP method involves the ranking of the indicators in the order of their importance in their contribution towards the aggregate index (*De*). The importance of indicator is measured by comparing the variability of the indicator with the aggregated index. Partial Least Square-Variable Importance in Projection Method (PLS-VIP) is a multivariate regression method where information from a data space of a larger number of variables is projected into that with a smaller number of variables. We start with the same data matrix, *X*as used to calculate the aggregated index. The indicators are the variables in the data space. PLS-VIP is a supervised model for which an overall data behavior or pattern is required. This overall pattern can be represented by a response vector or a response matrix. In our modeling we have used the aggregated index, *De* as the response vector.

In the PLS-VIP analysis, the number of indicators is reduced in a way such that variations in the set of reduced indicatorsare most likely to be reflected in the response vector *De*. In other words, the overall data pattern would be unchanged with the reduced number of indicators. The easiest test of this expectation is if one can make the same conclusions about the overall data behavior with this set of less number of indicators as was done with the original set. The surplus indicators would thus be understood to be redundant or not important in contributing to the overall performance of the system in question. An application of PLS-VIP for sustainability assessment has been given by Mukherjee et al. (2013). In multivariate method, there are variables which are inferred through a mathematical model of the original (observed) data and are known as latent variables. In contrast to the original variables, the latent variables are not explicit, nor can be tweaked at will. In this paper, the variables are the indicators, and henceforth, we will refer to the original variables as indicators, and the latent variables derived from the original indicators as latent indicators.

Partial Least Squares Regression (PLS) model is used to decompose the original data matrix X into two orthogonal matrices, the loadings (*L*) and scores (*T*) of *a* number of latent indicators, and a residual matrix, *E* as shown in Equation 3 (Cinar et al., 2004).

 (3)

The score matrix *T* is related to the response vector *De* through a regression matrix *b* as shown in Equation 4 (Chong and Jun, 2005). *F* is the residual vector of *De*.

 (4)

The values of the indicator for each option are represented as an option vector *xm*. Each option vector *xm* can be related to the score vector through weight vectors *wj* as given in Equation 5.

 (5)

The Variable Importance in Projection (VIP) for a particular indicator, is calculated using the regression coefficient *b*, weight vector *wj* and score vector *tj* as given in Equation 6.

 (6)

where *wkj* is the *kth* element of the weight vector *wj*.

PLS-VIP is used to identify the importance of each indicator in affecting the aggregate index *De*. In order to avoid the relative variability of the indicators to affect the result, normalized indicators are used for VIP calculation. This ensures variability within an indicator but avoid relative variability. Indicators with lower VIP scores have little influence on *De*, and those with the higher VIP scores contribute the most towards *De*. The average of squared VIP scores equals 1. VIP score greater than one is generally used as a criterion for detecting the relative importance of an indicator.

There are different algorithms available to solve PLS regression problems. In the present work, the regression for the PLS is based on PLS1 algorithm (Martens, 1991). In PLS1 algorithm, the correlation coefficient of *X* and *De* is used to obtain the first extracted score *t1* for the first latent indicator. After obtaining the first latent indicator, the regression follows by obtaining the second latent indicators from the residuals and so on. This is most appropriate for our problem where response matrix comprises of one column, constituting the aggregated indices, *De*. Regression coefficient and weight vectors from the first three latent indicator score vector are used for calculating VIP.

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