ISGC 2019
May 13th - 17th

N°582 / OC
TOPIC(s) : Life cycle and environmental assessment / Industrial chemistry

G2 - Greenness Grid to rank chemical products and processes

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PURPOSE OF THE ABSTRACT

Over the past few decades, chemists and engineers have made a strong effort to reverse the negative publicity associated to chemistry. [1] This negative stance results from the large amounts of waste generated by the chemical industries which is becoming increasingly expensive for the industry and the environment. Consequently, new topics such as Green Chemistry and Green Engineering have gained attention, as a way of encouraging people to develop ?green? solutions. This remarkable change in the world of chemistry was accomplished by REACH, the Registration Evaluation and Authorization of Chemicals, which has evolved into arguably the most important chemicals legislation to this day. [2]

Originally proposed in the 1991, green chemistry was used to describe the efforts of reducing pollution from chemical processes.[3] Later, Anastas et al. proposed guidelines to assess the ?greenness? of a chemical process, and established the 12 principles of green chemistry.[4] The main objective was to foster the development of green solutions that could reduce the waste [5], the carbon footprint [6], the potential toxicity [7], etc. Nevertheless, only 2 out of the twelve principles of green chemistry were supported by quantitative formulas, while the remaining were subject to qualitative interpretations, which from chemical and process points of view, generates unrealistic interpretations and comparisons.

In 1992, Life Cycle Assessment (LCA) was put forth as a technique that considers analyses of the environmental impact of a product's life cycle, from production to disposal.[8] However, it is an exhaustive tool since it requires a lot of data to accurate the values. Moreover, comparison between LCA's of different products/processes are not directly comparable. Recently (2017), De Vierno Kreuder et al, [9] described an approach to establish green chemistry metrics, that consists of evaluating chemicals and chemical processes against the 12 principles, using readily available data such as the data compiled in compliance with the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, the metrics Carbon Efficiency (CE), Curzons Reaction Mass Efficiency (RME) and Mass Productivity (MP) were not considered, and the values obtained for each principle weren't normalized for a direct comparison between principles.

The document herein, resulting of combined knowledge from areas with different scopes (chemistry, biology, energy, chemical process design, etc) presents a green chemistry grid (G2, greenness grid) to assess mathematically and objectively the greenness of a chemical product/process. The proposed methodology is composed by three important steps: (i) for each principle a set of formulae were proposed in order to obtain values that quantify the principle, (ii) new principles were proposed which involved CE, RME and MP, and (iii) all the values derived from each principle were integrated/normalized into values between 0 and 1 (where 1 represents the best scenario and 0 the worst-case scenario) applying transforming functions with the capacity to

integrate data that is updated over time, conferring a dynamic and versatile character to this tool. The selected functions were the regularized incomplete beta function [10,11] and the Kumaraswamy distribution's cumulative distribution function. [12,13]

Based on the score between 0 and 1 obtained for all of 15 principles, a green chemistry grid-G2, which varies from 0 (worst scenario) to 15 (best scenario), with a well-defined quantitative and qualitative scale was assembled, containing a final ?green index (Unsustainable Process [0-3[; Poor Process [3-6[; Average Process [6-9[; Satisfactory Process[9-12[; Green Process [12-15]) ? that allows transversal classifications of process/products from different areas or industries. The application of the greenness grid- G2 is described and demonstrated using a case study.

FIGURES

FIGURE 1
G2 - Greenness Grid
G2 - Greenness Grid

FIGURE 2

KEYWORDS
Green Chemistry Metrics | Green Chemistry Grid | Greeness Ranking | Sustainability

BIBLIOGRAPHY