Environmental Management

Proposal of a holistic environmental metric based on environmental indicators

Proposição de uma métrica ambiental holística baseada em indicadores ambientais

Guilherme Antonio Finazzi [I] iD **, Vivianni Marques Leite dos Santos** [I] iD

[I] University of São Francisco Valley, Juazeiro, BA, Brazil

ABSTRACT

There is no doubt Sustainability reaching is essential. Natural resources rational use is extremely important to human development. Beyond the years, this preoccupation led various institutions to elaborate legislation and international guides, as Kyoto protocol, to satisfy sustainability conditions. Agenda 2030 is the most recent instrument, whose proposals attempt to these conditions. Within this context, human activity related to Chemistry is noteworthy: to guarantee all sustainable aspects in a procedure is a great challenge. The assessment of Sustainability in Chemistry is performed by green metrics calculations, whose utility is most appropriate in comparison of procedures than in a single procedure assessment. Due to problematics with the utilization of metrics, related to: simplifications leading to pseudo-results, need of various misunderstanding calculations and incorrect adoption of metrics, an environmental metric that attempts to current necessities related to materials and energetics consumption and to assessment of sustainability in individual chemistry procedures is proposed. The metric was elaborated aiming to attempt all environmental requirements of chemical sustainability in a simplified and reliable manner, basing on bibliographic search and expertise. The metric elaboration has a combined approach, in which reference values are established to the main indicators of sustainability, using a Soft System Methodology (SSM).

Keywords: holistic environmental metric; Sustainable Chemistry; sustainability; Green Chemistry; Environmental Chemistry

RESUMO

Não há dúvida de que alcançar a sustentabilidade é essencial. O uso racional dos recursos naturais é extremamente importante para o desenvolvimento humano. Com o passar dos anos, essa preocupação levou várias instituições a elaborarem legislações e protocolos internacionais, como o protocolo de Kyoto, para

satisfazer as condições de sustentabilidade. A Agenda 2030 configura como sendo o instrumento mais recente de medidas propostas para atender a essas condições. Nesse contexto, a atividade humana relacionada à Química ganha destaque: garantir todos os aspectos sustentáveis em um procedimento é um grande desafio. A avaliação da Sustentabilidade em Química é realizada por cálculos de métricas verdes, cuja utilidade é melhor aproveitada na comparação de procedimentos do que em uma avaliação de procedimento único. Devido aos problemas da utilização de métricas, relacionadas a simplificações que geram pseudo-resultados, necessidade de numerosos cálculos mal-interpretados e adoção incorreta de métricas, neste artigo é proposta uma métrica ambiental que atende às necessidades atuais relacionadas ao consumo de materiais e energia e à avaliação da sustentabilidade de procedimentos químicos. A métrica foi elaborada com o objetivo de atender todos os requisitos ambientais de sustentabilidade química de forma simplificada e confiável, com base em pesquisa bibliográfica e experiência acadêmica. A elaboração da métrica possui uma abordagem combinada, em que são estabelecidos valores de referência para os principais indicadores de sustentabilidade, utilizando Soft System Methodology (SSM).

Palavras-chave: métrica ambiental holística; Química sustentável; sustentabilidade; Química verde; Química Ambiental

1. INTRODUCTION

From the industrial development in 18th century, the human activity has grown and, then, consequences to the environment and to people emerged. For example, the need of avoiding phenomena as the smog effect in London (LEIGHTON, 2012), thermal inversion at urban zones and industrial accidents, as at Bhopal (VARMA & VARMA, 2005), is due to the injuries caused to the population health. These effects emerged due to pollution caused mainly by Chemical Industry.

Concern with pollution led to mobilizations since Stockholm Conference in 1972 (UNITED NATIONS, 1972; SILVA, 2005). Solutions for problems related to pollution were (and still are) required. The major problem of Industry is the disposal of great amounts of waste generated at chemical procedures - that must be done without causing pollution (PRADO, 2003). Actually, in the past, due to difficulties in waste reduction, recycling was the only mean of prevention of the pollution by Industry (MACHADO, 2011), that is not sufficient to solver the problem, as it do not guarantee sustainability. Therefore, it was imperative to implement a new set of premises to bring to light the real necessity: the requirements for sustainable development (MICHELSEN, 2016; KÜMMERER, 2016).

Green Chemistry arose in this context, regarded the need of optimization of the procedures in Chemistry Industry, related to resources utilization, as well as to environment preservation. Through the years, the idea of sustainability in Chemistry evolved to the

concept of Sustainable Chemistry, that is beyond the simple prevention of pollution, as it involves all components for sustainability (MICHELSEN, 2016; KÜMMERER, 2016). The most recent instrument for goals elaboration in this matter is Agenda 2030 (UNITED NATIONS, 2015), whose objectives directly related to Sustainable Chemistry are:

- Guarantee sustainable production and consumption standards;

- Urgently act against climatic alteration and impacts.

Within this context, a reliable and simplified metric that attempts to the requirements for Sustainable Chemistry is necessary, regarding the evaluation within Agenda 2030 goals.

2. MATERIALS AND METHODS

This study was performed by an exploratory bibliographic research (CAUCHICK-MIGUEL, 2018), aiming to identify how the Green Chemistry Principles and some green metrics are employed in several research works and to evaluate the reliability of these criteria application regarding the sustainability concept. This article is divided in two sections: in the first, the identified problems related to the assessment in Green Chemistry are described and analyzed, regarding to misleading adoptions of green metrics and to the negligence of important aspects in sustainability evaluation.

In the second section, the proposal of an environmental metric for the assessment in Sustainable Chemistry is described, characterizing the work as an applied-normative study. The metric elaboration has a combined approach, in which reference values are established to the main indicators of sustainability, so that a Soft System Methodology (SSM) (CHECKLAND & POULTER, 2010) that attempts to as many as possible impactful factors in Sustainable Chemistry is performed.

The methodologic strategy for proposal of the holistic environmental metric (H.E.M.) was based on an exploration research of the principles of Green Chemistry, followed by an analysis of the traditional green metrics and culminating with the actual proposal.

3. RESULTS AND DISCUSSION

To identify approach problems or inadequate uses of the green metrics described in literature or both, an analysis of the Principles of Green Chemistry is necessary, considering the items: criteria for sustainability in chemistry; use of solvent and auxiliaries avoided or made innocuous; improvement in energetic efficiency; catalysts losses; relation between the principle of full mass balances with quantification and minimization of "utilities" use; relation between principle of basic thermochemistry investigation with principle of improvement of the measurement process in Sustainability (by development and application); and an analysis of traditional green metrics is also necessary.

3.1 Principles of Green Chemistry

The 24 Green Chemistry Principles established by Anastas & Warner (TUNDO et al., 2000; WINTERTON, 2001) and Winterton (WINTERTON, 2001; MACHADO, 2012), presented in Chart 1, aims a harmonic relationship between industrial production, consumption and quality of natural resources – dependent on all aspects of environmental conservation. However, it is important to consider that the elaboration of sustainable or "green" industrial procedures, mainly in substitution to older ones categorized as "red", "brown" or "black", is not trivial.

Chart 1. Green Chemistry Principles

Waste formation prevention

Atoms economy

Synthesis with low human toxicity and environmental impact

Product design with reducing toxicity

Auxiliary materials avoiding or making innocuous (including solvents)

Minimizing energy requirements

Use of renewable raw materials

Derivatization avoiding

Preference for use of catalyst

Degradability to innocuous chemicals

Avoiding hazardous materials formation by process monitoring

Process hazard and risk minimization by materials chosing

By-products identification and quantification

Conversion, seletivities and produtivities reports

Full mass-balance establishment for process

Catalyst and solvent loss measurement in effluents

Basic thermochemistry investigation

Prevision of heat and mass transfer limitations

Reactions visualization from engineers perspective

Consideration of the overall process effect on choice of chemistry aspects

Sustainability measurement improvement (by development and application)

Utilities quantification and minimization of use

Recognition of incompatibility between process safety and waste minimization

Laboratory waste monitoring, report and minimization

Source: Adapted from Winterton (2001)

Planning "green" industrial procedures requires previous studies and carefulness regarding to all experimental steps related to the search of sustainability at the processes. Besides, it is noteworthy to consider that the "production" of Industry wastes leads to additional costs to the sector, as it implies in new steps required to waste disposal, which can involve hazards, similarly to any fabrication step.

Then, the search of green processes really requires rigorous planning and previous and specialized expertise. This implies in the need of searching new processes alternatives and the carefulness to attempts to all Green Chemistry Principles is essential.

An example of green processes search is silicon oxide film solid phase extraction system development for lead traces quantification (COPELLO et al. 2011), accomplished with less solvents consumption and less waste production than traditional methods.

3.1.1 Criteria for sustainability in chemistry

The Principles of Green Chemistry is a list of factors that must be followed in the chemistry work. These factors are related to various criteria of sustainability, i. e., each individual principle does not attempt to an isolated criterion, nor comprises all ones. For example, considering environmental and human health impacts, four Green Chemistry Principles attempt these criteria: prevention of pollution; more safety synthesis; avoiding the use of solvent and auxiliary or making innocuous; use of catalyst (RIBEIRO et al., 2014). Then, even when regarding only these principles, the main Sustainable Chemistry objective must be taken into account: all criteria of sustainability must be satisfied. All action or evaluation must be grounded in the sustainability concept, even if it does not attempt clearly to the Green Principles established in literature.

3.1.2 Use of solvent and auxiliaries avoided or made innocuous (5th Principle)

There are solvents considered "greener" than traditionally ones, mainly regarding to Organic Chemistry procedures (SILVA, 2005). For example, ionic liquids are attractive due to low volatility and possibility of recycling, as they can be recovered for reuse (SKOUTA, 2009; CUE & ZHANG, 2009). Nevertheless, ionic liquids are not biodegradable, and are toxic to

some aquatic life species (KÜMMERER et al., 2019), even when recycled – what is viable only at large scale (SHELDON, 2000) –, because there are inevitable losses, whose fate is fatally the environment. Thus, their use is not yet the best choice in Green Chemistry practice, and not even in Industry, its use occurs at large scale (SHELDON, 2005).

Another example is supercritic carbon dioxide (SCD): this solvent is considered green, as it is atoxic, inert towards many substances, not flammable, and the fabrication is, at first, performed with atmospheric gas (SILVA, 2005; TUNDO et al., 2000; SHELDON, 2005; WARDENCKI et al., 2005). On the other hand, SCD can carry residues out of the chemical process to the atmosphere when volatilize, requires energy consumption to be fabricated and handled at elevated temperatures (WINTERTON, 2001; MACHADO, 2012; SHELDON, 2005), it is a greenhouse gas (TUNDO et al., 2000) and can be suffocating at large amount, leading to potential inconsistency with the search for sustainability. It is noteworthy to highlight the fabrication can occur from fossil fuels burning, distancing even more the use from the sustainability ideals.

In sustainability, procedures without solvents need are the best choice (SHELDON, 2005), as in the case of aqueous phase cobalt-nickel extraction using 8-hydroxyquinoline (SOROURADDIN et al., 2019), solid-phase extraction with ink-printed filter paper as adsorbent (VOULGARI et al., 2017), solid phase reactions (SHANKER et al., 2016).

3.1.3 Improvement in energetic efficiency (6th Principle)

Commonly, electric energy is produced with environmental impacts, notably by burning fossil fuels (LENARDÃO et al., 2003; MACHADO, 2014; SHELDON, 2018). Ideally, chemical reactions should occur at no energetic consumption or by means of non-pollution electric energy, e.g. produced by direct solar irradiation (TUNDO et al., 2000; AGEE et al., 2014). However, these means of production are not always available or efficient for chemical practice; therefore, electric energy is provided by traditional means. Thus, the maximum energetic economy is interesting when considering evaluation in Green Chemistry, if there is no mean of sustainable production of electric energy. Within this context, microwave oven and ultrasound bath uses are considered green (SILVA, 2005; PRADO, 2003; TUNDO et al.,

2000; VARMA, 1999). The main advantage of these technologies is the reduction of spent time in the procedure, reflecting in lower energetic consumption.

Another important factor related to the improvement in energetic efficiency is the accountings of energetic consumption of all devices used (e.g. related to heating mantle, Bunsen burners, etc), that is absent in some literature works. According to the principle of improvement of the measurement process in Sustainability (21th), these accountings are essential in the procedure of assessment in sustainability, due to associated costs and environmental impacts (WINTERTON, 2001; MACHADO, 2012).

3.1.4 Catalysts losses (16th Principle)

According to the 9th Green Chemistry Principle, catalysts must be correctly applied to obtain success, related to the increase in reactional yield at the same time span, as well as to minimization of waste generation (SILVEIRA, 2015). Nevertheless, uncritical use of catalyst is not always the best green alternative, as sometimes does not improve the chemical process greenness. For example, in transesterification reaction of recycled vegetable oil for biodiesel production, the increase in catalyst concentration causes an undesirable parallel reaction – saponification – in which transesterification catalyst also acts as a reagent, producing soap and water (MARTINEZ-GUERRA & GUDE, 2017).

Additionally, catalyst becomes a cumulative hazard waste if there are no recovering steps for posterior reuse (LENARDÃO et al., 2003; PUROHIT et al., 2017) and, then, its concentration must be measured (WINTERTON, 2001; MACHADO, 2012). In this case, green alternatives with low environmental impacts, as natural sugars (SOUZA et al., 2019), are interesting. Besides, it is technically simpler to recover an insoluble solid catalyst (heterogeneous catalysis), which is, in this point of view, greener than a soluble one (homogeneous catalysis) (SHELDON, 2005).

3.1.5 Relation between the principle of full mass balances (15th) with quantification and minimization of "utilities" use (22th)

Although water is considered a green solvent, ideal for reaction, isolation and purification steps (no doubt this is sustainable), for each chosen procedure, some or all waste is aqueous, and the entire amount of the aqueous waste generally is greater than the waste of solely the reaction steps (LENARDÃO et al., 2003). In particular, at biphasic catalysis with water, there is an inevitable solubilization of some compounds and solvents, even at low concentrations (SHELDON, 2005). In other words, water is a green solvent, but aqueous waste is not green in most cases. Thus, the amount of aqueous waste of the procedure must be entirely accounted in this way.

Another important aspect refers to the importance to consider both water used for cooling steps and gases used for inert atmosphere as waste, because they are discarded after all. Procedures considered "green" can spend too much water than the traditional ones (SHELDON, 2018), mainly when without entire water recover. Besides, the assessment upon only the reaction waste is not suitable, as there will be a negligence on the waste of other procedure steps, which implies in negligence of 15th and 16th principles of Green Chemistry (Chart 1) (WINTERTON, 2001; MACHADO, 2012).

There are other aspects that deserve attention, related to distillation steps and overflow accidents, in which inevitably solvents can volatilize to atmosphere (MACHADO, 2012; SHELDON, 2005) and then must be taken into account during assessment in Green Chemistry. Furthermore, it is important to highlight that this assessment must take into account the effects of those incidents in biota environment, as soil, rivers, lakes and other water bodies.

3.1.6 Relation between the principle of basic thermochemistry investigation (17th) with principle of improvement of the measurement process in Sustainability (21th)

In a procedure, the improvement in energetic efficiency can be reached by performing laboratory reactions at miniscale or microscale. Reducing size implies in better safety, e.g. decreasing the number of problems arising by the release of heat from exothermic reactions. Also, scale resizing of a chemical procedure defines the amount of the resources that will be used, including electric energy. Moreover, the amount of waste (e.g., in titrations with

econoburette (SINGH, 2011)) and the consumption of electric energy in microscale is lower than in macroscale (MACHADO, 2012).

3.2 Traditional green metrics

To assess the "greenness" of chemical processes, green metrics were elaborated. Machado (2014) classify green metrics in: mass metrics, which involves mass values of chemical compounds of a procedure; energetic metrics, which involves values of energy consumption of a procedure; environmental metrics, related to sustainability assessment (environmental benignity) at various scales; and economic metrics, related to involved costs (HEINZLE et al., 1998). Except regards to the last one, a discussion about the use of the main metrics is realized as follows:

3.2.1 Adoption of mass metrics and energetic metrics

Usually, each mass metric is too useful to assess amounts of waste and reaction yields, whereas each energetic metric is too useful to assess energetic consumptions, being both metrics attractive in the point of view of Industry. The possibility of economy with reducing amounts of waste and energy consumption, in addition to increase in reaction yields, is the base of Industry profits. Nevertheless, this kind of assessment is merely economic: mass metrics measure only atomic productivity (RIBEIRO & MACHADO, 2012); e.g., E-factor and PMI do not assess toxicity of waste (RIBEIRO et al., 2010a). An example of misleading use of these metrics refers to the results of the assessment of biodiesel synthesis, that led the authors to infer that the synthesis with methanol is greener than with etanol (MARTINEZ-GUERRA & GUDE, 2017), as the metrics included only factors related to yield (involving only the mass of the final product), neglecting characteristics of methanol, as toxicity and non-renewability.

In short, assessment by isolated metrics or by metrics adopted arbitrarily - without proper theoretical basis - is an unreliable practice, as denominate some procedures as green, even when various criteria for sustainability are neglected, e.g. the environmental ones (RIBEIRO et al., 2010a; RIBEIRO & MACHADO, 2011; CONSTABLE et al., 2002).

3.2.2 Environmental metrics

A manner for preventing problems with the choice of mass metrics is the association with sutainability indicators that envolve risks related to human health and environmental impacts, e.g. environmental quocient (Q-factor) (SHELDON, 2018) and Scale Risk Index (SRI) (DUARTE et al., 2017), (based on the Globally Harmonized System of Classification and Labelling of Chemicals - GHS (UNITED NATIONS, 2019). These metrics are not frequently used due to the problem of precision in determining values associated with those impacts. Furthermore, they do not include all possible environmental impacts of each chemical compound, so a broader metric concept is necessary.

3.2.3 Search for a holistic metric

With the efforts in a way to establish a most suitable parameter for environmental assessment, utilizing green metrics, several authors started to consider algorithms for metrics calculation (DUARTE et al., 2017; CALVO-FLORES, 2009; AZAMBUJA, 2013; LESEURRE et al., 2014; PHAN et al. 2015; EISSEN & METZGER, 2002; AKEN et al., 2006; OWSIANIAK et al., 2014; BARE, 2011; GOEDKOOP & SPRIENSMA, 2001; ECKELMAN, 2016), as well as graphics (RIBEIRO et al., 2010a; RIBEIRO et al., 2010b; CALVO-FLORES, 2009) to represent a holistic metric. An alternative that most closely matches to an appropriate holistic metric is Life Cycle Assessment (LCA) (ISO, 2006a; ISO, 2006b), as it takes into account the environmental factors associated with sustainability, e.g. Global Warming Potential (GWP), Eutrophication Potential (EuP), Energy Consumption (EC).

LCA is a tool that can properly guide an assessment in sustainability, as it accounts all essential aspects in a "cradle to grave" manner, i.e. since the extraction of each substance from nature, up to its final disposal. In practice, LCA is a set of submetrics calculated upon data obtained by chemicals emissions. However, assessing the life cycle of a compound can be very complicated, as it involves various variables in the calculation (AZAMBUJA, 2013; OWSIANIAK et al., 2014; BARE, 2011; GOEDKOOP & SPRIENSMA, 2001; ECKELMAN, 2016), as well as relationships of life cycles of other compounds (MACHADO, 2012), similarly to several metrics involving algorithms (RIBEIRO et al., 2010a; RIBEIRO et al., 2010b; CALVO-

FLORES, 2009; LESEURRE et al., 2014; PHAN et al. 2015; EISSEN & METZGER, 2002). The entire assessment of LCA is not easy, as it takes into account various factors to obtain a reference value for each submetric (GOEDKOOP & SPRIENSMA, 2001). Furthermore, there is a need in adapting the methods and models of LCA according to some local characteristics, e.g. of South America (MENDES, 2013).

Among the alternatives found in the research, involving the algorithms or use of graphics for metrics representation, there are metrics that result to a simple number: a single reference value for assessment of the "greenness" of chemical processes (RIBEIRO et al., 2014; RIBEIRO & MACHADO, 2012; AKEN et al., 2006). In these cases, the assessment procedure and the comparison between different procedures are extremely easiest. However, they do not seem suitable to assess the sustainability of chemical procedures: most calculations and graphics are performed based on a simplistic (sometimes arbitrary) pontuation, as adopted in some other works (DUARTE et al., 2017; PHAN et al. 2015, EISSEN & METZGER, 2002), attributed to factors directly associated to some principle of Green Chemistry or any environmental impact factor, without accounting specificities and concentrations of chemical compounds (RIBEIRO et al., 2010a; RIBEIRO et al., 2010b).

3.3 The holistic environmental metric (H.E.M.) proposal

The H.E.M. described as follows was elaborated aiming to attempt all environmental requirements of chemical sustainability in a simplified and reliable manner as possible, i.e. a Chemical H.E.M. But, at first, a method to perform properly the assessment is essential and must be described.

3.3.1. Initial method of assessment

To begin an assessment study in Sustainable Chemistry, the establishment of the boundaries for the chosen procedure is required. An independent reactional procedure, or a separated purification step, or a procedure that envolve both or more steps can be analysed.

The boundaries definition determines the ultimate result of the assessment. In some cases, the desired final product is the mixture of all substances after the reaction finishes; so, an assessment process on sustainability will differ from another accounting isolation and purification steps. For example, the assessment of the entire procedure of tris-acetylacetonate-cobalt(III) synthesis or potasium nitrilosulfonate synthesis is different compared with that performed without isolation and purification steps (MACHADO, 2014; DUARTE et al., 2014).

If the desired product must be isolated and purificated, performing assessment on sustainability without take into account those steps is not satisfactory, as some particular aspects are not involved. The results of this practice is a differenciated but misleading assessment: processes accounting in only reaction steps seem "greenner" than processes accounting also posterior steps, although in both cases the reaction procedure is the same.

Ideally, the boundaries of the overall procedure must be the broadest as possible, i.e. sustainability assessment must involve all transformation steps, since extraction of impure reagents from nature towards products and final disposal of waste back to source. However, due to difficulties in accomplish such a comprehensive inventory, mainly referring to an industrial process (MACHADO, 2007), the procedure boundaries may be established by considering the use of reagents and solvents and posterior steps, involving "auxiliaries", until the purification oh the desired (final) product, including analytical characterization and waste generation.

It is important to highlight that making the analytical characterization a less polluter procedure is a Green Chemistry challenge. Depending on the method, performing this step will generate a great amount of waste. Therefore, before chosing the analytical method, previous analysis of environmental impacts of potential waste is essential (WARDENCKI et al., 2005).

Afterwards, all involved aspects at the delimited procedure and all amounts must be inventoried, without exception (CONSTABLE et al., 2001). Chart 2 shows an example of an inventory.

Chart 2: Inventory of items involved in a chemical procedure.

Stage	Procedure /Step	Specificity	Item	Quantity/ value	Total	Unity	Observations
Initial, intermediary (ies) or final	Preparation Reaction Purification Isolation etc.	Defines each material or energetic resource role: reagent (limitant or in excess), auxiliary, product, waste, renewabilit...	material or energetic resource	(for each experiment execution)			

Source: Authors (2021)

If some input values are not directly available, each missing data can be calculated or estimated. By analysing reaction yields, the amounts of all wastes, i.e. excess reagents, coproducts and original impurities, can be calculated or estimated.

With the amounts of all utilized materials, the mass balance of the procedure can be carried out and calculating or estimating solvents losses is possible. For example, the calculation of the flow rate of liquids is a tool for calculating or estimating solvents losses; knowing the power of an electric device and its operating time, energetic consumption can be calculated or estimated.

There are other important aspects regarding to the inventory. First, energy obtained by burning fuels must be accounted not only related to energetic consumption, but also to the impacts of the fuel and the combustion reaction, including waste generation. Second, the differentiation between "desired products" and waste must be made, as "desired products" are chemical compounds of interest that are effectively purified during the delimited procedure, when appropriate. Non-purified products and coproducts of the reaction, even when have interesting applications, must be considered as waste, if they are not the target. For example, in transesterification of recycled vegetable oil (MARTINEZ-GUERRA & GUDE, 2017), although glycerol can be used, e.g. as cosmetics, it is waste, if is not effectively recovered as a product.

Third, after reaction proceeded, catalysts are always waste, and must be accounted in this manner. If catalyst can be recycled, the environmental impacts will not be the same as for a non-recycled one (MACHADO, 2014), as the fate of the last will be fatally the environment. In other words, the environmental impacts of a catalyst are lower when it is 100% recycled, since they may be computed only at the last performed procedure, while a non-recycled catalyst has a cumulative effect at each procedure.

Fourth, gases emisions may be calculated with pressure and temperature data, and solvents losses by evaporation can be estimated by analysis of evaporation rate, whose data can be found in literature, e.g. Saboia (2010), or by laboratorial measures. If reactional losses by evaporation occurs and are non-computing, the amount of waste will be lower than in

the case of full mass balance (15th principle of Green Chemistry) (WINTERTON, 2001; MACHADO, 2012), leading to an equivocated assessment.

An example of the evaporation rate influence in the assessment result is the case of methanol and ethanol evaporations in biodiesel synthesis (MARTINEZ-GUERRA & GUDE, 2017). As methanol is more volatile, its losses can be greater than ethanol ones; then, the amount of liquid waste in the former case can be lower, which may lead to a false conclusion that it is greener.

Fifth, as mentioned before, the use of water - for example, at distillation and reflux cooling (WINTERTON, 2001; MACHADO, 2012) - is important in waste accounting. Though it is a green solvent, sometimes the disposal in water bodies is not appropriate, due to differences in temperature (VERONES et al., 2010). Moreover, water used in chemical procedures is usually from human supply, and then has the same requirements of treatment that for comunity offering.

A problem related to water supply is the employment of an available technology with low cost to make feasible its treatment and distribution, since water becomes an expensive resource at scarcity periods (RIJSBERMAN, 2006; MEKONNEN & HOEKSTRA, 2016). Thereby, the use of water also has impacts in Sustainable Chemistry, and then must be included in the assessment.

Sixth, biological processes are too complex to perform a detailed and actual analysis by identifying and quantifying the reaction products. Some examples are process of obtaining agricultural biomass (MACHADO, 2012), domestic or organic compounds wastewater treatment (TCHOBANOGLOUS et al., 2003), in which analysis are carried out by COD and BOD measures (MEENACHI & KANDASAMY, 2019).

In these systems, the controll of formation of chemical compounds and the account of all aspects of the inventory are complicated, as involve many chemical reactions and, therefore, many reaction products. Thus, a proper assessment of these systems must be estimated by using data of previous studies in literature. Besides, according to Kümmerer et al. (2019), some recently detected chemical species, as their transformation products, are not included in the assessment, due to difficulties in quantification, as they are at concentrations

below the environmental quality standards, when these standards exist. In these cases, the maximum hazard (lower sustainability) associated to these materials must be accepted (DUARTE et al., 2014).

Seventh, and finally, quantification of waste depends on its storage or disposal forms or both. When segregated, the concentrations of the chemical species are greater than in the case of all waste in a single flask. Thus, detailing the waste storage or disposal forms or both at the inventory is very important.

3.3.2 H.E.M. calculation

The proposed Holistic Environmental Metric (H.E.M.) is based on environmental indicators (submetrics) used at LCA calculation, taking also in account the principles of Green Chemistry and the basis of some commonly mass metrics (WINTERTON, 2001; STRANDDORF et al., 2005). One main objective at the proposal was the establishment of reference values that are available in literature as tolerance limits for each indicator. Some of these values were defined according to the classification criteria described in GHS (UNITED NATIONS, 2019).

To accomplish the metric calculation, initially all the inventory data (Chart 2) are used in submetrics calculation. All aspects must be considered: reagents, waste, energy, reaction yield, etc. Besides, the database or the dataset used for these calculations must be referenced.

Fifteen submetrics were established as follows. The submetrics unities are not always from SI, due to difficulties that would arise in the calculations.

3.3.2.1- Problematic of Prevention on Waste Generation.

To assess the amount of waste with environmental impacts of a procedure, the calculation of the quantity of all waste is needed, discounting those included in any category as follows:

•	Materials storaged for reuse or effectively recycled, not discarded (total mass m_{rr});

• Materials disposed appropriately: purified materials whose disposal was executed in the same place that the chemical compound was extracted from nature, and that does not represent environmental pollution as it is disposed (total mass m_{tad}) or

• Degradable materials that are not storaged for reuse nor recycled: accounted only when are segregated from non-degradable waste (total mass m_{tdr}), otherwise they would present human health or environmental risks.

An individual chemical species may not be included in more than one listed category, avoiding recounting and overestimated results.

Then, the submetric Problematic of Prevention on Waste Generation (PPWG) is calculated by equation (1).

$$PPWG = 100\% - \left(\frac{\sum(m_{tr}) - \sum(m_{rr}) - f \times \sum(m_{tad}) - \sum[(m_{tdr}) \times f_t]}{(\text{total mass utilized directly at the procedure})} \right) \times 100\% \tag{1}$$

m_{tr} is mass of total waste;
f is the factor that represents the depretiation of pontual concentration of all in natura material at the disposal place, due to the increase caused by proper disposal; total mass utilized directly at the procedure does not include discarded tapping or purified water (e.g. distilled, deionized, etc.);
f_t is the degradability factor of each chemical compound, given by:

$$f_t = \frac{28}{t_d} \tag{2}$$

t_d = delay (in days) to degradate 60% of total mass of the chemical compound (immediate biodegradability, according to OECD (1992)).

3.3.2.2- Exposure to Toxic Compounds.

In this submetric (ETC), the toxic compounds contents are considered, according to the equation:

$$ETC = \frac{1}{e} \times \sqrt[e]{\prod \frac{E_e}{C_{re}}} \times 100\% \tag{3}$$

E_e is the maximum ideal exposure to the analysed toxic compound, given by

$$E_e = C_{te} \times t_e \ (g \ kg^{-1}h) \tag{4}$$

C_{te} is the limit concentration of toxicity, i.e. the limit value of the concentration that represents toxicity of the compound, that is expressed by mass of compound to kilogram of exposed individue ratio ($g.kg^{-1}$), or compound concentration in solution (converted to $g.kg^{-1}$ using density values at 1 atm and 25º C);
t_e is the exposure term (measured in hours) in an assay for determination of C_{te} (when not available, te is assumed to be 1)
C_{re} is the concentration of the chemical compound in the waste;
e is the number of toxic compounds in the waste.

Each value of E_e must be the minor within the assays data, i.e. the minor exposure to the compound that brings risks to fauna or flora or humans or all life. Also in case of human health hazards, inhalation exposure to particulate matter must be considered, when wastes are storaged in solid form ($PM_{2.5}$ or PM_{10}).

There are some important aspects to highlight. The first is the possibility of misunderstandings regarding to the choice among toxicity data, as it is different depending on the country/region (RIBEIRO et al., 2014; SHELDON, 2018; CONSTABLE et al., 2002; MORITA & MORIKAWA, 2011; DOMÈNECH et al., 2002). Besides, there are limitations about toxicity information of many known substances (DUARTE et al., 2017). Ideally, the limit concentration of toxicity must be the maximum NOEC value (no observed effect concentration) available in literature; however, this value will not always be accessible. To avoid these problems, the use of the minor value available (e.g. of MATC, CE_{50}) is proposed, all found preferably at PubChem database (NCBI, 2021). In exceptional cases, data found at the specific Material Safety Data Sheet (MSDS) of the substance or mixture may be used (RIBEIRO et al., 2014).

Furthermore, even an apparently innocuous substance, as sodium chloride, can be problematic as waste, depending on quantity (SHELDON, 2000); e.g. if a disposal of the salt at the soil occurs, there is a possibility of crops harming by decrease in plant nutrition (PEDROTTI et al., 2015). Thus, one compound is considered innocuous only when been below its limit concentration of toxicity.

3.3.2.3- Accumulation of Toxic Compounds

Accumulation in biota (ATC) is determined by:

$$ATC = \frac{1}{a} \times \sqrt[a]{\prod \frac{1}{f_a}} \times 100\%$$

(5)

f_a is an accumulation factor of the toxic compound, e.g. bioconcentration factor (BCF) or bioaccumulation factor (BAF) or n-octanol/water partition coeficient (K_{ow}) (CRONIN & LIVINGSTONE, 2004), which may be found in literature or at the specific Material Safety Data Sheet (MSDS) of the substance or mixture (RIBEIRO et al., 2014); a is the number of compounds with the same kind of factor.

The value of the submetric must be the minor as possible, and must be calculated utilizing only one kind of factor, which must be mentioned. Values until 1 must not be considered. For pure metals and metallic ions, f_a must be related to exposure at concentration C_{te} or above, as is dependent on it (DeFOREST et al., 2007).

3.3.2.4- Human Carcinogens and Mutagens.

Ideally, the assessment of carcinogenesis and mutagenicity (HCM) must involve minimum concentration values and term of exposure to hazardous substances.

However, due to data missing at the literature, the life cycle inherent toxicity value of exposure to dimethyl carbonate synthetic route, utilizing fosgene and methanol via methylchloroformiate, i.e. 769 cases per kilogram of individue at inhalation exposure (ECKELMAN, 2016) was adopted as reference value to all substances. So, the submetric is calculated by the equation:

$$HCM = \left(\frac{1}{769}\right)^m \times 100\%$$

(6)

m is the number of substances with mutagen or carcinogen potential, which may be found at IARC database (WHO, 2021) or at MSDS.

In absence of any substances with human mutagen or carcinogen potential, HCM is equal to 100%.

3.3.2.5- Procedure Safety.

The assessment of all safety parameters of the procedure (PS) is given by

$$\text{PS} = \sqrt[n]{\prod \frac{1}{f_n \times C_{rn}}} \times 100\% \tag{7}$$

f_n is the safety risk factor of the chemical compound;

C_{rn} is the concentration of the chemical compound at the procedure, in g mL^{-1};

n is total number of chemical compounds utilized.

f_n is calculated for each chemical compound of the procedure. In the calculation, the risks of potential hazardous reactions for each participating chemical are included, i.e. after all, the risks are accounted as many times as the number of the chemicals in each hazard reaction. The factor is composed by 5 safety risk components, as follows:

$$f_n = f_e \times f_p \times f_f \times f_g \times f_c \times \frac{1}{N} \tag{8}$$

1. f_e is the risk factor of potential explosion, equal to:
     - the propagation speed of the potential explosion, in m s^{-1}; or
     - the gas volume produced by gram of explosive at the potential explosion, in mL g^{-1}, when there is no propagation speed data; or
     - 9000 (equivalent to the highest explosion propagation speed recorded in the literature, in m s^{-1}, when the anterior data are missing) (OXLEY, 1998); or
     - 1, when there is no potential risk of explosion.
2. f_p is the risk factor of confined gases pressure (cases of potential explosion or implosion), given by:

$$f_p = \left(\frac{n_g \times P_v}{P_{atm}} \right)^x \tag{9}$$

n_g is the number of mols of the gas, that can be estimated by Gas Laws;

P_v is the vapor pressure of the gas, i.e. the pressure that the gas assumes at confinement (high when compressed, low when in vacuum);

P_{atm} is the atmospheric pressure at the environment; x is:

- +1 for compressed gas risk, or

- -1 for vacuum risk (to identify high or low pressure situation, confer GHS) (UNITED NATIONS, 2019).

f_p = 1, when there is no potential risk of confined gas pressure.

Note: aerosols must be included here, so that their pressure must be estimated.

3. f_f is the risk factor of potential fire, determined in flammable, pyrophoric and self-heating substances cases (according to classification in GHS (UNITED NATIONS, 2019)), as:

- $f_f = H$

$$\text{(10)}$$

Where:

H is a process enthalpy, e.g. combustion enthalpy (complete or partial), dissolution enthalpy, neutralization enthalpy or others. They are calculated or estimated by theoretical values or measured (values in J g^{-1}), or

$$\text{(11)}$$

- $f_f = \dfrac{1}{LEL}$

LEL is the lower explosive limit, given by absolute volume/volume ratio LENTINI, 2013). This value is adopted when determination of H is not possible; or

$$\text{(12)}$$

- $f_f = \dfrac{366}{FP}$

FP is the flash point (in K) of the compound; the calculation is accomplished in enthalpy and LEL missing data cases. The value 366 K (i.e., 93°C) is associated to maximum flash point to consider a liquid flammable, according to GHS; or

- ff = 1, when there is no potential risk of fire.

4. f_g is the factor related to potential formation of oxidizing atmosphere or toxic gases emissions due to fire or both. Its value is

$$\text{(13)}$$

$f_g = \dfrac{V_g}{m}$

i.e. the produced gases amount V_g by reagent mass m ratio, in mL g^{-1}. f_g equals 1, when there is no potential risk of oxidizing atmosphere formation or toxic gases emissions due to fire or both. Except in specific cases, V_g

calculation is carried out with the environment temperature, considering negligible its change at the overall environment at the beginning of reaction.

5. f_c is the corrosion factor, given by:

$$f_c = \frac{1}{6.25} \times \frac{\Delta M}{\Delta t}$$
(14)

- $\frac{\Delta M}{\Delta t}$ is the maximum rate of corrosion of steel or aluminium at 55°C by the chemical compound, in mm year^{-1}; or
- $\frac{\Delta M}{\Delta t} = 10 \times V_{corr25}$, where V_{corr25} is the maximum rate of corrosion of steel or aluminium at 25°C by the chemical compound, in mm year^{-1}; or
- f_c must be 1 when there is no evidence of corrosivity;

6.25 is the reference value of corrosion rate in mm year^{-1} (UNITED NATIONS, 2019).

6. N is the number of utilized items for prevention on safety at the procedure, such as personal protective equipment, exhaust hood, controlled environment chambers, etc.

Some substances with the anterior characteristics are listed at United Nations Economic Comision for Europe (UNECE) site and the main guidelines criteria are listed at GHS file (UNITED NATIONS, 2019), from the same institution. The codes for these substances from GHS are H2XX, and X varies from 0 to 9. Data may be found preferably at PubChem database (NCBI, 2021) or at the specific Material Safety Data Sheet (MSDS).

3.3.2.6- Catalysis Efficiency.

When reaction is catalysed, this submetric (CE) is given by:

$$CE = \frac{(\textit{non-catalysed reaction term}) - (\textit{catalysed reaction term})}{(\textit{non-catalysed reaction term})} \times 100\%$$
(15)

Reaction term, in seconds (s), is the total time for chemical reaction(s) occurrence, when there is(are) reaction(s). When no catalysis occurs, CE = 0.

(Continue...)

3.3.2.7- Electric Energy Consumption.

In this submetric, the electric energy consumption (EEC) is related to final product mass:

$$EEC = \frac{(worldwide\ daily\ average\ electric\ energy\ consumption\ per\ capita) \times (product\ mass)}{(total\ non\text{-}renewable\ daily\ average\ energy\ used\ at\ the\ procedure)} \times 100\% \tag{16}$$

Product mass (purified, when is the case) is expressed in kilogram (kg);
energy values are expressed in quilowatt-hour;
the value of worldwide daily average electric energy consumption per capita may be found in literature (IEA, 2021), referencing the year of collected data.

The spent energy at the procedure should comprise energy values from fuel burnings, due to Bunsen burners and utilization of similar devices (MACHADO, 2012). These values must be estimated on experimental data or on literature or on both. It is noteworthy to highlight that the daily renewable energy consumption at the procedure is not accounted in this submetric, as it attempts to 7th Green Chemistry Principle.

The calculation of equation (16) is accomplished when the worldwide daily average electric energy consumption per capita is not numerically greater than the total non-renewable daily average energy used per kilogram of the product at the procedure. For the other cases, EEC = 100%.

3.3.2.8- Global Warming.

The global temperature increase of the planet (GW) due to increase in greenhouse gases concentrations (e.g. carbon dioxide) is accounted for:

$$GW = \frac{(total\ mass\ utilized\ at\ the\ procedure)\text{-}\sum CO_2\ equivalent\ mass}{(total\ mass\ utilized\ at\ the\ procedure)} \times 100\% \tag{17}$$

CO_2 equivalent mass is:
- the gas mass liberated on the process, corrected by GWP factor according to AR5 (WRI & WBCSD, 2021); or

- Total carbon dioxide mass that would be released at waste treatment (including incineration steps) by each compound in the waste.

3.3.2.9- Ozone Layer Depletion Potential.

The ozone amount depletion at stratosphere due to reaction with chemical compounds (OLDP) is expressed by:

$$OLDP = \frac{(total\ mass\ utilized\ at\ the\ procedure) - \sum CFC\text{-}11\ equivalent\ mass}{(total\ mass\ utilized\ at\ the\ procedure)} \times 100\% \qquad (18)$$

CFC-11 equivalent mass is:

- CFC-11 mass released at the process, or
- gas mass released at the process, corrected by ODP factor (SOLOMON & WUEBBLES, 1995).

When any material storage relative to the procedure involves refrigeration use, refrigeration gas losses must be taken into account. In case of missing data, CFC-11 equivalent mass losses can be estimated by 0.01425 g of HCFC-141b per hour. This standard is defined based on 1.0 liter of HCFC-141b loss (most utilized gas in refrigeration) in 10 years.

3.3.2.10- Smog Photochemical Formation.

The main reason of smog formation (SPF) is the increase in ozone amount at the troposphere, due to reaction with chemical compounds, and is expressed by:

$$SPF = \frac{(total\ mass\ utilized\ at\ the\ procedure) - \sum ozone\ equivalent\ mass}{(total\ mass\ utilized\ at\ the\ procedure)} \times 100\% \qquad (19)$$

as:

$$Ozone\ equivalent\ mass = smog\ former\ gas\ mass \times (MIR)$$

$$(20)$$

and MIR is the upper limit correction factor for each potential smog photochemical former gas, found in literature (CARTER, 2000a; CARTER, 2000b).

3.3.2.11- Acidification Potential.

Substances with hidroxon release potential (acidificants) contribute to this submetric (AP), expressed by:

$$AP = \frac{(total\ mass\ utilized\ at\ the\ procedure) - \sum (acidificant\ mass \times SO_2\ equivalent)}{(total\ mass\ utilized\ at\ the\ procedure)} \times 100\% \tag{21}$$

SO_2 equivalent is a conversion factor, in g, for acidificant mass (STRANDDORF et al., 2005), given by

$$SO_2\ equivalent = 32.03 \times \frac{mols\ of\ H^+\ released\ per\ mol\ of\ acidificant}{acidificant\ molar\ mass} \tag{22}$$

3.3.2.12- Eutrophication Potential.

Nutrient enrichment (EP) allowing plankton and algae proliferation in water depends on nitrogen and fosforous environmental disposal (STRANDDORF et al., 2005).

To perform the submetric calculation, initially nitrogen and fosforous in waste must be quantified, to evaluate which nutrient is in excess in EP contribution, according to nitrogen/fosforous molar ratio of 16:1. Thus, the total content of the nutrient in excess is used for calculation, as represents maximum eutrophication potential. Calculation is described in equation (23):

$$EP = \left(\frac{(total\ mass\ utilized\ at\ the\ procedure) - \sum NO_3^-\ equivalent\ mass}{(total\ mass\ utilized\ at\ the\ procedure)} \right) \times 100\% \tag{23}$$

NO_3^- equivalent mass is total mass of the nutrient in excess in the waste (m_{exc}), in g, corrected by a factor (c) related to each nitrogen or to each fosforous compound:

$$NO_3^-\ equivalent\ mass = m_{exc} \times c =$$

$$= m_{exc} \times 62 \times \sum \left(compound\ mass \times \frac{number\ of\ N\ or\ P\ atoms\ in\ the\ compound\ formula}{compound\ molar\ mass} \right) \tag{24}$$

3.3.2.13- Consumption and Disposal Thermic Potential of Water.

As mentioned before, water must be treated as waste, as by CDTPW:

$$\text{CDTPW} = \left(\frac{7 - V}{7}\right) \times \frac{|T_{air/environment} - T_{water/environment}|}{(|T_{discarded\ water} - T_{water/environment}|)} \times 100\%$$

(25)

V is total daily volume of consumed water at the procedure, in m^3;

$T_{air/environment}$ is the air temperature of the environment, at the procedure, in K;

$T_{water/environment}$ is water temperature without heating or cooling steps, in K;

$T_{discarded\ water}$ is the temperature of the water at disposal moment, in K.

The reference value of 7.0 m^3 hab.$^{-1}$ day^{-1} is the water daily need per capita, added to consumption estimation for daily agricultural production per capita (BASTIAANSSEN & STEDUTO, 2017).

If *V* is greater than 7.0 m^3 hab.$^{-1}$ day^{-1}, CDTPW is considered zero. Consider 0.01 K for the difference between $T_{discarded\ water}$ and $T_{water/environment}$, when it is below this value.

3.3.2.14- Human Health Damage caused by Ionizing Radiation.

Radioactivity influence on human health is related to mutagenic diseases, cancer and even death. Equation (26) involves its calculation:

$$\text{HHDIR} = \frac{1}{r} \times \sqrt[r]{\prod \frac{7.5}{s_{(r)r} \times m_{r(r)r}}} \times 100\%$$

(26)

r is the number of distinct radionuclides in the waste;

$s_{(r)r}$ is the radionuclide specific activity, in Bq g^{-1};

$m_{r(r)r}$ is the radionuclide mass in the waste, in g, that must be calculated with the relative natural abundance regarding to the respective element.

Values can be obtained at International Atomic Energy Agency site (IAEA, 2008) and at IUPAC reference (HOLDEN et al., 2018). Value of 7.5 represents natural radioactivity of a 70 kg human body, in Bq.

Only values of ($s_{(r)r} \times m_{r(r)r}$) above 7.5 are accounted in the calculation. In total absence of radionuclides, HHDIR = 100%.

3.3.2.15- Resources Consumption.

This submetric calculation (RC) is performed by:

$$RC = \frac{\sum m_{tcd}}{(1-\alpha) \times m_{enup}} \times 100\%$$

(27)

m_{tcd} is the mass of materials disposed correctly: whose disposal was executed in the same place and at the same manner that the chemical compound was extracted from nature, i.e. the chemical compound is returned exactly as was extracted;

m_{enup} is total resources extracted from nature and utilized in the procedure, that can be estimated;

α is the renewable to total resources ratio, defined by Dewulf et al. (2000).

Ideally, all submetrics values must be between 0% and 100%. But for some submetrics calculation, negative values as well as values above 100% can be obtained. In these cases, consider 0% and 100%, respectively. Although this issue, without making a relashionship with a reference value – a standard – getting problems dimension of each procedure is not trivial, even when accomplishing a direct comparison to the standard or in a fixed parameter absence case. For example, it is difficult to identify the problem extension of procedures comparing its mass intensity (MI) value directly with the maximum experimental value of 18377, for (–)-huperzine A (MACHADO, 2014).

The ideal H.E.M. calculation involves all fifteen submetrics. Besides, if there is some datum missing for any submetric calculation, the environmental risk associated to this datum is assumed to be maximum (DUARTE et al., 2014). The proposed H.E.M. calculation may also be accomplished by the means as follows:

1) Reductionist mode. Only submetrics 1 to 5 are involved in this form, which may be applied when there are difficulties in data obtaining for calculation of submetrics 6 to 15, due to failing in structure for assessment, e.g. for fine chemicals and intermediates LCA at the pharmaceutical industry (SHELDON, 2018; DOMÈNECH et al., 2002). Although there are discrepancies about classifications regarding chemicals toxicity (RIBEIRO et al., 2014), its absence in the assessment cannot be justified, as toxicity affects all life maintenance, i.e. it is against Sustainability.

2) Guided mode. Includes calculations of reductionist mode, and also submetrics 6, 7, 13 and 14.

3) Expanded mode. All submetrics are calculated from the delimited procedure inventory, except those related to nature resources extraction (submetric 15).

4) Exhaustive mode. All submetrics are calculated from the delimited procedure inventory, without exception.

To facilitate the visualization of the calculated values, the submetrics set is expressed in a figure, similarly to a previous described in literature (RIBEIRO et al., 2010a; RIBEIRO et al., 2010b). In this article, the figure has a bar graph form, called green graph, as at following Figures 1 and 2:
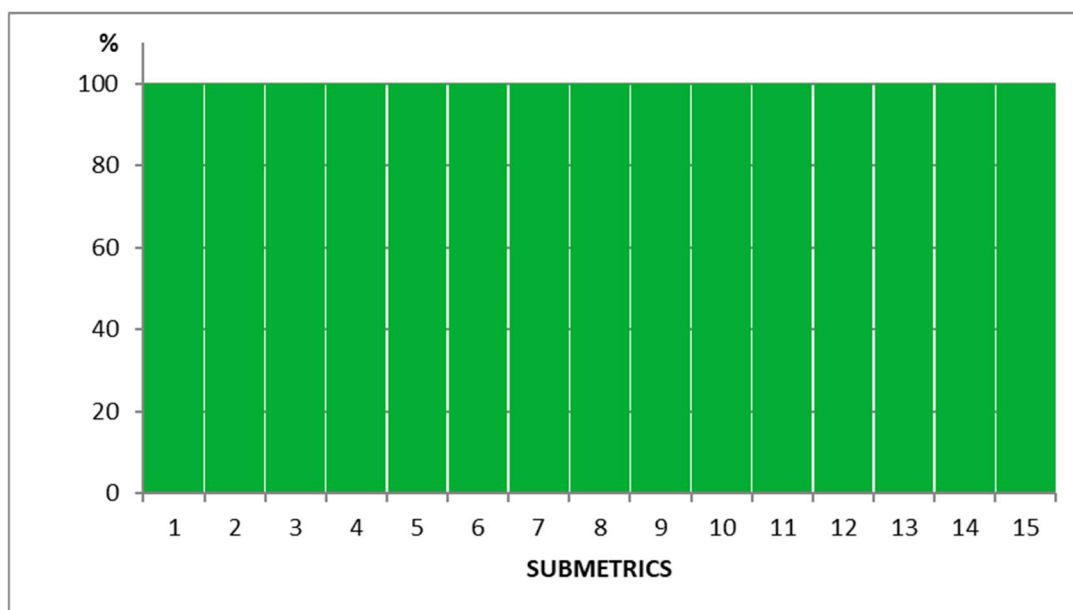
Figure 1: Graph presenting submetrics values at a procedure without sustainability
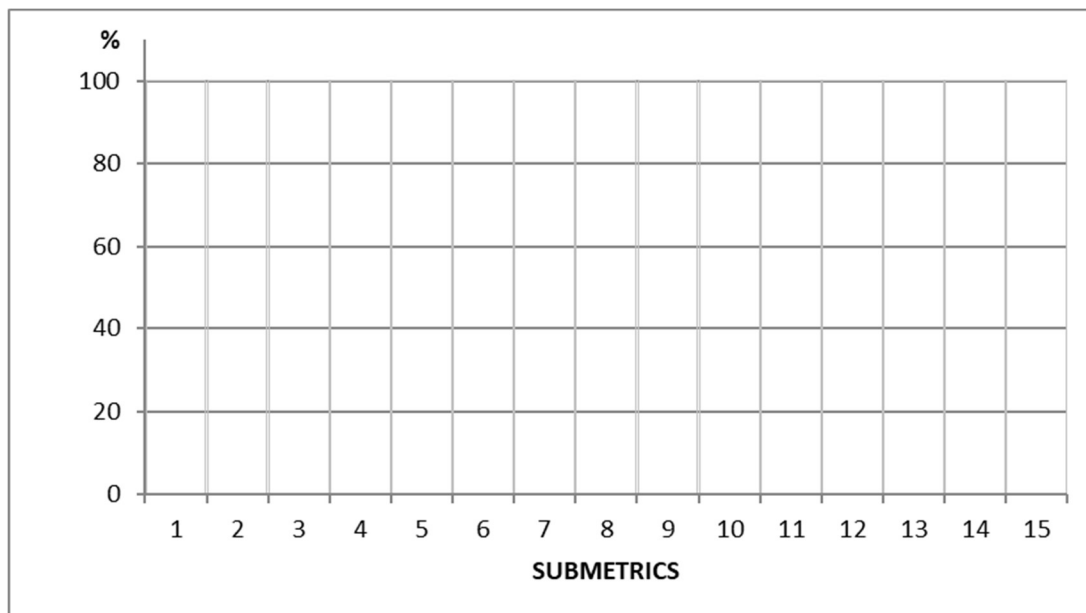
Source: Authors (2021)

(Continue...)

Figure 2: Graph presenting submetrics values at a fully sustainable procedure (Green Graph)

Source: Authors (2021)

The H.E.M. is calculated considering the procedure dimensioning, related to the final product amount, in g, and the exposure term to all procedure characters:

$$H.E.M. = \frac{submetrics\ aritmetic\ average\ value}{(final\ product\ mass) \times (exposure\ term)} \quad (28)$$

For an easiest and fastest process assessment, a computer program that implement the metric calculation is been developed, called SCASys (Sustainable Chemistry Assessment System).

3.3.3 Metric relation with Green Chemistry Principles

In Chart 3, relation between the proposed metric and Green Chemistry Principles is presented.

(Continue…)

Chart 3. Relation between proposed metric/submetrics with Green Chemistry Principles.

Principle	(Sub)metrics	Principle	(Sub)metrics
1	1, 13	13	1
2	1	14	1*
3	2, 3, 4, 8, 9, 10, 11, 12, 14	15	1
4	2, 3, 4, 10, 11, 14	16	1
5	1, 5, 13	17	5
6	7	18	5
7	15	19	All and H.E.M.
8	1*[1]	20	All and H.E.M.
9	6	21	All and H.E.M.
10	1, 3	22	1, 13, 15*
11*	2, 3, 4, 5, 8, 9, 10, 11, 12, 14	23	1, 5
12	2*, 4*, 5, 14	24	1, 2*, 3*, 4*, 8*, 9*, 10*, 11*, 12*, 13, 14*

*Indirect form
Source: Authors (2021)

As shown in Chart 3, the proposed metric can be related to all Green Chemistry Principles, corroborating to reliability of the H.E.M. regarding to sustainability.

4 CONCLUSION

In this article, a holistic environmental metric (H.E.M.) based on LCA and on Green Chemistry Principles was proposed. The metric calculation was developed with environmental indicators, for which were established reference values as standards, to perform sustainability assessment in a more reliable and simplist manner as possible, i.e. without too simple pontuations or extensive algorithms. The H.E.M. advantage is the coverage of all Green Chemistry Principles, avoiding conflicts that may arise with

equivocated metrics adoption. H.E.M. calculation allows similar procedures comparison with the same product obtaintion aiming, as comprehends values between 0% and 100%. H.E.M. accounts the environment requirements set for sustainability in addition to exposure term to the procedure and its dimensioning, related to final product mass. In addition, a computer program is been implemented for calculating the metric to conduct the assessment in a fastest and easiest manner, so that speeding up data analysis can be reached, enhancing its applicability.

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APPENDICE

In the supplemental material, the H.E.M. calculation of copper electrodeposition from baths containing dissolved copper salt or digested copper alloy is presented.

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AUTHORSHIP CONTRIBUTIONS

Guilherme Antonio Finazzi
Chemistry
https://orcid.org/0000-0002-8369-6140 | guilherme.finazzi@univasf.edu.br
Contribuition: Conceptualization, Visualization, Writing – original draft.

Vivianni Marques Leite dos Santos
Chemical Engineering
https://orcid.org/0000-0001-8741-8888 | vivianni.santos@univasf.edu.br
Contribuition: Conceptualization, Writing – review & editing.

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