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Evaluation method for process intensification alternatives

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ABSTRACT

A method for the comparison of scenarios in the context of Process Intensification is presented, and is applied to cases reported in the literature, as well as several examples taken from selected industrial practices. A step by step calculation of different factors, all relevant in the chemical engineering and cleaning processes is also given. The most important feature of this new method is the simplicity of arithmetic operations, and its robustness for cases where there is limited information to provide a good assessment. The final calculated value, the Intensification Factor, provides an interesting decision-making element that can be weighted by experts, no matter which level of detail or the particular activity is considered (economical, technical, scientific). Additionally, it can contain as many quantitative and qualitative factors as there are available; they are all lumped into a number with a clear meaning: if larger than one the new alternative is superior to the existent; if is smaller than one, the opposite applies. The proposed method is not to be considered only as a tool for experts in the specific process intensification discipline, but as a mean to convince outsiders. Also, it can be used in educational settings, when teaching young professionals about innovation and intensification strategies. A discussion forum has been created to evaluate and improve this method and will be open to professionals and interested researchers that have read this paper.

1. Introduction

Decisions are regularly taken, either in the scientific, industrial or commercial activities, in order to find optimal conditions, re-design an equipment towards overall plant performance improvement, purchase new technology, and other situations. Maximising profit is usually the reason for doing any of the above listed tasks. When a new technology or product is considered for the substitution of an existing one, it is necessary to compare both considering specific aspects. Perhaps the biggest difficulty found in most cases is the integration of various technical, economic and environmental indicators, as well as quantitative and qualitative information. Most existing methods found in literature have a wide range of complexity and transparency; which strongly determines whether its practical implementation is feasible, or adopted with less resistance by the specific industrial sector or scientific community.

1.1. State-of-the-art in Process Intensification and evaluation methods

Process Intensification concepts (PI) have gained attention in disparate chemical engineering activities. Its goals are related to new, sustainable and efficient ways for the manufacturing of chemical products [1]. In short, innovative principles in both process and equipment design are introduced as long as they can lead to significant improvement in process efficiency, product quality, and reducing waste streams. Naturally, the decision of "intensifying" a process, which means changing something in the existing plant or technology, demands a deep analysis and rigorous decision process [2]. PI strategies can vary depending on the field of chemical engineering besides PI, such as Process System Engineering (PSE), where different approaches have been identified: Structure (spatial domain), Energy (thermodynamic domain), Synergy (functional domain) and Time (temporal domain) [1]. In the same paper, the following principles have been postulated: (a) maximizing the effectiveness of intraand

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Fig. 1. New classification of process intensification and Problem representation according to Ponce [4].

intermolecular events; (b) giving each molecule the same processing experience; (c) optimizing the driving forces and maximizing the specific areas to which these forces apply; (d) maximizing synergistic effects from partial processes. These principles and approaches can be applied at different scales, from the molecular processes, passing through microfluidics, to macroscale (reactors), and up to the megascale (plants, sites, enterprises) [3].

Process integration strategies can be useful for intensifying process in a broader concept related to PSE, e.g. modelling, optimisation, control, etc. [4]. In the cited paper, a division into two categories has been made: unit and plant intensification. A mathematical formulation for each intensification process was proposed (see Fig. 1) considering the intensification of existing units as well as the installation of new ones. The applicability of this model was presented in the same paper cited, as a very elaborated case study that we also employ later in some examples given (Section 3.5).

The challenge in designing sustainable processes due to scarce information, and in a format that can be understood by both chemists and engineers has been previously identified [5]. Inspired by green chemistry principles [6], techno-economic analysis and environmental lifecycle assessment, a methodological tool was proposed for early stage multi-criteria assessment and used in the evaluation of key process development decisions for novel production of renewable fuels and bulk chemicals [7]. Existing in-depth analyses tend to be based on data difficult to collect and consume significant amounts of time, particularly when referring to downstream processing, normally unknown during early design phases of laboratory or scaling-up [7,5]. There are professional softwares and qualitative assessment techniques such as Aspen Icarus Process Evaluator, E-factor, GME, EcoScale, ProSuite, BASF eco-efficiency and the Sustainability Consortium Open IO that help in such calculations. Most of these methods are information intensive, and require time and resources for its collection [5,7].

The method we introduce in this work, was initially designed to make comparisons particularly in academic settings, and later was expanded for real-life scenarios. In a first approximation, there is no need to include cost considerations (as normally is the case in academic settings), yet, as demonstrated in several cases in this paper, it can be easily added to assist in a decision-making process, where reliable and time-efficient assessment at different stages of a project are of relevance. This method is a simple evaluation tool that could provide a relatively fast assessment in the form of a "number" to allow the discussion in a team of experts, or to convince "outsiders" of the benefits or drawbacks of a new proposed chance. This method is not intended to be used for optimisation in the current form, which requires proper validation and is out of the scope of the present study. Such validation can be possible if relevant and sufficient data of existing plants is made available, and a proper long-term study can be carried out to evaluate whether the implementation of the intensified solution was indeed better. We look forward to research or innovation teams that would like to join efforts in this respect in the future.

Economical constraints are the main hurdles for the adoption of any new project. In practice, there are difficulties in quantifying the "improvement" of independent factors not necessarily interrelated or connected to cost. This is also the case when trying to combine "qualitative" aspects such as (perceived) safety, overall impression, e.g. better-worse. An index defined as the ratio of the total costs of raw materials used in the process with respect to the value of all the marketable products and co-products at the process end, has been identified as the simplest, yet incomplete approach for assessing the economic viability of chemical processes [8]. This index is one component of a screening method based on a multi-criteria approach allowing quantitative and qualitative proxy indicators for the description of economic, environmental, health and safety, as well as operational aspects tailored for an integrated biorefinery concept. The authors have defined the following indexes: EC, Economic constraint; EI, Environmental impact of raw materials; PCEI, Process costs, and environmental impacts; EHSI, Environmental-Health-Safety index; RA, Risks aspects. These categories could be evaluated as part of an early-stage sustainability assessment as favorable or unfavourable with respect to its petrochemical counterpart.

Other authors have proposed a complementary view of PI based on the concepts of local and global intensification [9]. Local PI stands for the classical approach based on using techniques and methods that improve drastically the efficiency of a single unit or device. The drivers of local PI are primarily technical (maximizing the production of a compound, e.g. goals) although there are other "drivers" as efficiency, cost, ecological impact, productivity or yield. Their proposed global method focuses on the calculation of the efficiencies for different extensity values of units or steps. Similarly, a multi-objective decision framework relying on data available at early design stages was introduced before [10]. It includes reaction mass balances, raw materials and products prices, environmental impacts of the life-cycle as a cumulative energy demand (CED) and greenhouse gas (GHG) emissions of the feedstocks, physicochemical properties of reactants and products, as well as existing hazards [5]. This method was adjusted for the production of bio-based chemicals, after including pretreatment of biomass, distribution of environmental burdens by product allocation, number of co-products, risk aspects and comparing processes with the petrochemical equivalents. It has five sustainability indicators: economic constraint (EC), environmental impact of raw materials (EI), process costs and environmental impact (PCEI), Environmental-Health-Safety index (EHSI) and risk aspects (RA); which are lumped into a score index with weighting factors that provides a comparison between all process alternatives. For the calculation of this index, scores are normalized by the worst score of the two processes under comparison. Weights based on the opinion of experts are assigned taking into account economic feasibility on a commercial scale; long term sustainability together with environmental impacts as low as possible; short term or immediate hazards; and risk aspects for decision makers. Summing the normalized values for all indicators yields a single index or total score for both processes under analysis, which are later compared by its ratio. For values < 1 the new (bio-based process) provides benefits over the traditional (petrochemical). Other methodologies for the local (classical PI) or global (whole process simultaneous improvement of several units) intensification have been reported,

demonstrating the richness and complexity of this topic [11].

As discussed before, the integration of technical and non technical (commercial-cost, safety, etc.) types of factors is a difficulty many engineers and scientists have faced. This might be the reason why many have prematurely abandoned PI solutions. In this paper, we present a method to calculate a single "number or value" which shares elements of existing indexes or methodologies, but is simpler than those we found in literature.

As will be seen in the several examples given in the following sections, we apply the proposed method and illustrate how it can be used by experts. Particularly, we see a great relevance as a tool in the process intensification discipline. The method has also been tested for two consecutive years as part of the Process Intensification Principles course that one of the authors teaches at the University of Twente. Taking the students as "outsiders", the explanation of this method, and its application in academic settings has shown certain advantages. The most important, is that they come to realise how difficult is to take decisions when faced with choosing among innovation or intensification strategies, specifically when there is more than one solution to a particular problem.

The strongest feature of our proposed Intensification Factor (*IF*) is its simplicity in arithmetic operations, and the possibility to get a "value" even when detailed information is not available at early or advanced stages in a project. As it will be seen in the following sections, this tool can be used in combination with already existing methods, expanding the toolbox and methodologies engineers and scientists require. After presenting the method, we provide several test cases and discussions to illustrate how the method can be applied in practice in Section 3.

2. Material and methods

The *IF* is composed of modular interchangeable evaluation criteria or factors (*F*). A convenient aspect is the possibility to combine qualitative and quantitative factors. We envisage this *IF* number as a tool that can assist in the decision making process at different levels, such as at the laboratory when researchers try to compare one setting or feature change, at the plant or equipment level in PI or PSE, but also at the managerial, consumer/commercial level. The individual factors can be as many as needed, or based on the available information. We consider that with this approach there is no "focusing limit" for the application of this tool; it can be applied at all scales in the PI strategy, e.g. molecules, structures, unit, PSE, etc, and there is freedom to couple the qualitative aspects to costs when required.

2.1. Method and Formulation of the tool

In a hypothetical plant, there can be different processes, units or even independent equipment needing intensification or improvement of any of its parameters. A given *F* can be the operation time, the yield of a given reaction, or the residence time through a reactor to allow a reaction to occur. For a given factor *F*, we have as input data its initial value F_b , the value after the modifications F_a . An exponent will serve our method in two ways: first, the sign will be determined whether a decrease or increase in F is beneficial; second, its absolute value will be taken as a weight factor that will depend on its importance with respect to the final goals of the intensification strategy (details will be given later). Table 1 illustrates the steps and required values in order to

 Table 1

 method steps to calculate IF.

Factor	Before	After	Exponent	Fraction
F	F _b	F_a	d	$\text{IF} = \left(\frac{F_b}{F_a}\right)^d$

obtain an individual impact factor IF.

For simplicity during the explanation of the method, the exponent d in the cases described in this paper will be taken as follows (except when noted):

$$d(F) = \begin{cases} +1 & \text{if a decrease in } F \text{ factor is desired} \\ -1 & \text{if a decrease in } F \text{ factor is undesired} \end{cases}$$

The meaning of the absolute value of d needs to be determined depending on the intensification target. For example, if safety, cost or commercial considerations, have a stronger relevance for the decision makers, experts would have to agree on its value. If such information is not available or agreed by experts, it can be set to unity as we have assumed for almost all the case-examples presented in Section 3. The intensification factor for a given number of n changes can be calculated as follows:

$$IF = \prod_{i=1}^{n} \left(\frac{F_{b_i}}{F_{a_i}}\right)^{d_i}.$$
(1)

From a mathematical point of view, an almost obvious limitation of this method can be found when a zero value appears at the denominator (gives 'infinite' value), or annulation if on the numerator. In practice this limitation can be circumvented. For example, where Temperature or Pressure values are used which in some scales can reach "zero", a different scale could be used (converting from Celsius to Kelvin).

Besides these simple limitations, the selection of F_i values needs further attention. The challenges in the selection of scales, and how to measure quantities has been a topic of debate for many years; particularly in the cases of changing scales where the sign of a specific value can pass through zero [12]. If we take the scale of a physical quantity (e.g. temperature or pressure) and change it in a linear way:

$$F_i = p_i \cdot F'_i + q_i \tag{2}$$

for example, the parameters p_i and q_i could be used to change from Celsius (*F*) to Fahrenheit (*F'*) scale, such that the former affects the ratio of the scales, while the latter determines the offset between the scales. It is easy to demonstrate that the ratio of F_i (before and after) defined in our method holds only if there is no offset between the scales, this means $q_i = 0$. It can be concluded then that the computed IF value will depend on the use of scales for quantities in the Intensification Factor. Consistent outcomes will be obtained only for scales chosen in a way that they have an absolute zero level. Ratio scaling does not impair the outcome for IF; however, having an offset between two scales for the same physical quantity, will render our method useless. The use of an interval for a performance variable is also a valid way to compare *F* values, because the effect of the offset will drop out when taking the length of an interval as the difference between its end and its beginning.

Independent IF_i values can be calculated for each possible change (e.g. longer channel, different material, improved safety, or ecological impact, economic benefits, etc.), for a given equipment or process under analysis for its improvement or replacement. The total *IF* of a global intensification initiative having a number of potential intensification strategies *p* can be calculated as

$$IF_{total} = \prod_{i=1}^{p} (IF_i)^{c_i}.$$
(3)

This new c_i exponent serves the purpose of giving different levels of importance to independent factors, and their actual value should be agreed upon before any computational use of our simple method. At the beginning of a project, when the information available is limited or non existent, the value of each c_i can intituively be set to one; this IF_{total} we consider it as the "base case". If the experts decide that safety and environmental impact factors are more important than cost or maintenance, a consistent assigning of the exponents can be made such that the higher the importance of the IF, the higher the exponent $c_i \ge 1$. If the information to assign individual values is available *a priori*, or as the

project advances, the corresponding values should be updated. The base case then can be used to compare the newly calculated values resulting from the progress made in the project. For the remaining of this work, we have assumed the base case in all instances.

For example, if a column reactor is changed for a smaller and compact alternative, and at the same time a heat exchanger is placed close to the reactor to use rejected heat and improve heat transfer efficiencies, the total intensification factor IF_{total} can be calculated as follows (an example is given in Section 3.6).

$$IF_{total} = \prod_{i=1}^{2} IF_i = IF_{column \ reactor} \cdot IF_{heat \ exchanger}.$$
(4)

A step-by-step procedure utilising the proposed method is illustrated in Fig. 2. The objectives and weights need to be found, depending on the particular situation. In those cases that performing an experiment is not possible, or lack of data do not permit the "after" assessment, the experts should guesstimate and reach a consensus. For example, the variables or factors could be specific variables associated with economy, safety, control, etc.

3. Results

In the following sections we will provide a number of cases to illustrate the way to apply the method described above, a discussion of these cases is given in Section 4.

3.1. Oscillatory baffle reactor

The oscillatory baffle reactor (OBR) was introduced as a novel form of continuous plug flow reactor, where tubes are fitted with constriction orifice plate baffles equally spaced [13]. The baffles are shaken in an oscillatory manner (range 0.5–10 Hz), in combination with the flow of the process fluid. It has been employed for the conversion of a batch saponification reaction to continuous processing that resulted in a 100-fold reduction in reactor size, greater operational control and flexibility (see Fig. 3).

The greatest driver for making this a continuous processing reaction was safety because continuous operation could reduce considerably solvent inventories. Furthermore, operating at a lower temperature of

(Step 1. Select Objectives)

F factors, parameters based on drivers (efficiency, profit, eco-impact, ...). This defines the Fb values. Define exponent d value based on desired/undesired increase of F.

(Step 2. Establish broad context)

Societal, economical, ecological, ... Ensure good quality of source, credibility, ... Re-assess parameters from Step 1 based on new Intensification solution, Re-assessment defines Fa values (if no experiment available), If experiments are possible, obtain empirical Fa values.

(Step 3. Apply IF Method)

Considering empirical or guestimated Fa, and Fb

(Step 4. Select most relevant IFi values

Rank IFi considering empirical or guestimated Fa, and Fb If possible, split in a) Technically feasible, b) costs, commercial potential, etc.

(Step 5. Propose Intensification Solution)

Make a forecast based on Steps 1 and 2.

If no experiment available in Step 2, make experiment for validation.

If Step 2 was based on experiments, decide to continue or not with Intensification.



Fig. 3. Saponification reactor system as presented in [13]. With permissions from Ind. Eng. Chem. Res., Vol. 40, No. 23, 2001.

85 °C, closer to the ambient pressure boiling point of the solvent, had a positive impact in safety. This new temperature could also be associated to energy savings, combined with improved heat transfer of the new reactor design. Among the several advantages, the size reduction helped decreasing the residence time, operation costs and down-time. A conceptual industrial-scale unit, with 20-pass, 500 l OBR has been reported to produce continuously at a rate of 2 T/h assuming 15 min mean residence time .

The factors used for the *IF* calculation of this test-case are Temperature, Pressure, Volume and Residence time, which are listed in Table 2. Since a decrease in Temperature is desired, the *d* value is taken as positive. We have assumed that a decrease in pressure is desired due to safety and costs, that is why the *IF*_{pressure} is less than one and it decreases the *IF*_{total} value. But a new *IF* number could be calculated to assess how much better would it be to operate at a higher pressure if desired (d = -1), for example when the reaction kinetics would benefit from it. Similarly, for Volume and Residence time the *d* value is 1, since is desired to work with less inventories.

The final *IF* is 19.44 > 1 meaning that the new proposed reactor has

Fig. 2. Step-by-step procedure that can assist in the decision making of whether intensify or change a given process. Particularly in Step 2 is where the weight factors should be identified or agreed by experts.

Test case of an oscillatory baffle reactor (OBR) taken from literature [14].

Factor	Batch	OBR	d	Fraction	IF _{total}
Temperature [K] Pressure [bar] Volume [m ³]	388.15 2.013 75	358.15 171.013 0.5	1 1 1	$(388.15/358.15)^1 = 1.08$ (2.013/ $171.013)^1 = 0.012$ $(75/0.5)^1 = 150$	
Residence time [min]	120	12	1	$(120/12)^1 = 10$	19.44

an overall positive performance. If desired, we could have added a "Safety" driver, for which experts would need to assign values for each alternative; either based on available experimental data or based on an arbitrary scale. The strength of this "value" will be more evident when we compare in other examples more than one alternative (see Section 3.3).

3.2. Sono-micro-reactor and Cavitation Intensification Bag reactor

Several chemical and physical effects caused by ultrasound are a result of cavitation, the formation and collapse of bubbles in a liquid exposed to oscillating pressure fields [15]. These type of reactors are widely used in laboratories and industrial applications, but the analysis and comparison of results obtained with them are notoriously difficult, which has limited the scaling up of sonochemical reactors in industry [16-18]. We present here two types of reactors in which the use of artificial microscopic crevices (which can be considered as a PI-Structure modification) improved the energy efficiency values for the creation of radicals [19-21]. The new bubbles created with ultrasound emerge from the artificial crevices and provide a larger amount of radicals together with several other phenomena. Sonochemical effects such as radical production and sonochemiluminescence were among the intensified aspects. The energy efficiency value X_{US} is calculated as the product of the energy required for the formation of OH· radicals and the rate of radical production, divided by the electrical power input. With three small crevices or pits, 10 times higher energy efficiencies were reached in a micro-sono-reactor (μ SR) [19]. The same principle was scaled-up, now labeled Cavitation Intensification Bag (CIB), and applied in the operation of conventional ultrasonic bath technology having ~900 crevices [21]. The μ SR and CIB concepts can be seen in Fig. 4. The CIB holds a volume 25 times bigger than the μ SR, and provided a reduction of 22% in standard deviation of results. The variability of sonochemical effects is a serious issue to be solved for its appropriate commercialization in industrial settings. More important,

Table 3

Table 4

Energy efficiency $\times 10^{-6}$ [–] of having Pits or not in a μSR [19] and CIB using two different ultrasonic devices (US₁ and US₂) [21].

Case	No. pits	Pits	d	Fraction
μ SR	1.6	9.1	$ \begin{array}{r} -1 \\ -1 \\ -1 \end{array} $	$(1.6/9.1)^{-1} = 5.69$
CIB with US_1	1.8	2.5		$(1.8/2.5)^{-1} = 1.39$
CIB with US_2	3.3	4.7		$(3.3/4.7)^{-1} = 1.42$

Test case for the CIBs for cleaning of jewellery and 3D prin	ted narts

Case	Factor	Conventional	Bubble Bags	d	Fraction	IF _{total}
Jeweller	Time [min] Volume [L]	10 3	2.5 0.05	1 1	$(10/2.5)^1 = 4$ $(3/0.05)^1 = 60$	240
3D part	Time [min] Volume [L]	8 100	1 50	1 1	$(8/1)^1 = 8$ $(100/50)^1 = 2$	16

an increase of 45.1% in energy efficiency compared to bags without pits was achieved.

In Table 3 we compare three scenarios; the first is the microreactor at the highest power with the largest number of crevices (three) against the unmodified reactor [19]. The other two comparisons are modified and non-modified bags for two ultrasonic baths (US) with different frequencies and power settings [21]. Comparing both USs is a useful feature of this method that cannot be easily carried out otherwise [23]. The exponent *d* is negative in all cases since higher X_{US} is desired.

From these values we can observe that the highest intensification of radical production is achieved by the microreactor alternative. For the CIB cases, the apparently simple comparison among types of CIB, with and without pits when CIB in US_2 has more energy efficiency overall. But our method becomes more important when looking at the different baths and using the CIB (with pits and without) by calculating the *IF*. Looking at the final fraction, the comparable values means that the CIB with pits have an *IF* ~ 1.4, and is independent from the US bath used. This is a very useful way to compare different intensification approaches.

Other ways to illustrate the advantages this method with the same CIB (commercially known as BuBble Bags) is for cleaning applications. It has been reported that the Bags are efficient in the cleaning of 3D printed parts that need to be cleared of the support material, cleaning of microfluidic chips, and jewels in commercial settings [24–27]. In Table 4, two examples are given for the calculation of the improved

Fig. 4. Overview of the setups for the experiments (left) with the μ SR [19,20] and the CIB (right) [22].





effect (*IF*) of using the CIBs quantified by the time needed for cleaning and the volume of liquid required for it. The first factor has a direct relationship with costs where the second has an additional environmental positive connotation, since the use of less liquid (containing detergents, or expensive solvents) has a smaller environmental footprint. These numbers are of great importance for the evaluation and quantification of cleaning, which has been reported to be not only difficult, but of industrial relevance [28]. With these numbers it could be also possible to compare different cleaning methods and equipment, in settings or activities outside of the academic interest.

3.3. Organometallic reaction in fine chemical and pharmaceutical industry

Up to this case we have compared only between two alternatives. This case offers the opportunity to compare among three different alternatives, for which we compare 1 vs 2, 1 vs 3 and 2 vs 3. Three different scenarios were compared for a campaign producing 5 tons of an isolated intermediate through a multistage organometallic reaction (see Fig. 5) [29]. The first scenario is the standard where the reaction is performed batch-wise, with six batch assets of equal size in series, each performing a specific task (protection, Li-exchange, coupling, hydrolysis, extraction and distillation). The slowest step becomes the bottleneck which is the coupling reaction because it takes place at cryogenic temperatures to avoid side-product formation. The second scenario is a mix of continuous and batch processing, having the Li exchange and coupling reactions performed in a microreactor at the expense of an additional investment. As a consequence, the reaction temperature is increased to avoid long residence time, resulting in an increase in the overall yield (from 75% to 80%) and throughput for the coupling reaction (from 1.7 to 2.1 kg/min). In this case, distillation is the bottleneck instead of the coupling reaction, but the workup operations (extraction, distillation, centrifugation, and drying) remain the same. In the third scenario, labeled as process synthesis design (PSD), all reaction steps are made in continuous-flow operation, which has the advantage of further reducing the batch assets and the number of operators, nevertheless, higher additional investment is required. It is assumed that there is not further gain in yield and throughput.

In this process the yield is preferred as high as possible because the cost of raw material is the dominant operating costs. The next largest cost is manufacturing, so the number of operators is preferred to be as small as possible, while throughput as high as reachable (to decrease operating time). We observe that a global IF based on those factors gives a simple indication of the reduction in operating costs, and therefore, increase in economic gain. We asume that any necessary additional investment, when annualised, is negligible compared to the former operating costs. When comparing the 2nd and 3rd alternative

against 1, it is evident that 3 has higher IF value (2.27), corresponding to a better intensification of the whole change if 2 would be selected (1.62). This is quantified by 2 vs 3 calculation, where an IF of 1.4 is the result. Clearly, the larger IF value the higher the economic gain that is finally achieved, which is in agreement with the economical gain reported by [29]. In a practical situation the number of factors might be much higher, and the possibility of talking about single numbers (IFs) can be much more helpful in the decision making process. Only factors with the largest impact on the chosen figure of merit should be selected. The multiplicative nature of the factor F implies that after comparing case 1 vs 2 and 1 vs 3, it is not necessary to compare 2 vs 3. Hence, in practical situations such an extensive table might not be of use (or required). For clarity purpose we have decided to include the three situations.

3.4. Dynamic disadvantages of intensification in inherently safer process design

From a study reported elsewhere [30], Portha et al. [10] analyse several cases, from which we took an example to demonstrate another advantage of our simplified method. It has been argued that a direct link between intensified process and inherent safety is not always true. A global analysis of the process should be performed instead because small hold-ups could be sensitive to disturbances causing rapid changes within the process. As a result, safety and product-quality constraints would be affected before corrective actions are put in place. To select just one example, the comparison of benzene nitration in two alternatives scenarios, with the same objective of 96% conversion is taken here (see Fig. 6). The first scenario is a large CSTR whilst the second one having two small CSTRs, each reactor is equipped with a cooling jacket.

When dynamics considerations are not included, the intensification principles would favour the two small reactors scenario, since the reduced inventory of dangerous materials and more compact and smaller equipment can be converted into lower capital cost and also less coolant; the latter due to larger cooling heat flux per reacting volume of the reactor (higher surface to volume ratio and temperature difference). An increase to 120% and decrease to 80% with respect to the nominal value of 100% was calculated by the response of each configuration to a step in the benzene flow. Larger temperature deviations were found for the intensified scenarios due to the lower heat thermal capacity of the smaller reactors, which implies less robust process for dampening the heat released in the reaction. The relevant factors in this case having a d = 1 are the Volume, and Temperature deviations since they are all desired to be smaller in the intensified version (see Table 6).

The original analysis made by the papers cited above can be contrasted with the calculated IF = 0.52, which means that the Intensified

Fig. 5. Three different scenarios of commercial production using a multistage organometallic reaction, (1) batch, (2) continuous-batch, (3) Process synthesis design; adapted from [29].





Fig. 6. A large CSTR compared with a second scenario having two small CSTRs (modified from [30]).

Test cases for organometallic reaction [29]; assumptions and economical gain for scenarios in commercial production, assuming the current Gain is 100% for the Batch case (1).

Case	Factor	В	Α	d	Fraction	IFtotal
1 vs 2	Yield gain [%] Operators [–] Throughput [kg/min]	100 3.5 1.7	105 2.8 2.1	-1 1 -1	$(100/105)^{-1} = 1.05$ $(3.5/2.8)^{1} = 1.25$ $(1.7/2.1)^{-1} = 1.24$	1.62
1 vs 3	Yield gain [%] Operators [–] Throughput [kg/min]	100 3.5 1.7	105 2 2.1	-1 1 -1	$(100/105)^{-1} = 1.05$ $(3.5/2)^1 = 1.75$ $(1.7/2.1)^{-1} = 1.24$	2.27
2 vs 3	Yield gain [%] Operators [–] Throughput [kg/min]	105 2.8 2.1	105 2 2.1	-1 1 -1	$(105/105)^{-1} = 1$ $(2.8/2)^{1} = 1.4$ $(2.7/2.1)^{-1} = 1$	1.4

alternative seems not to be better than the current large CSTR. If the maximum temperature deviations that are allowed in order not to affect process safety and product quality were known, the final decision could be taken on a more justified basis. For instance, if the maximum temperature deviation observed in intensified case (3.6 °F) had negligible effect on process safety or product quality, the temperature deviation factor would be irrelevant in the comparison (or in other words, d = 0 for temperature deviation).

From a philosophical and moral perspective, we are of the opinion that in cases such as the one just described, the value of the weights emerges as an important tool. A higher weight value could be given to those intensification factors that contribute to a higher safety, compared to those having an emphasis on the process performance. Since the assigning of values to given weights can only be possible by experts in the specific process, we prefer not to speculate about this.

3.5. New understanding and systematic approach

We base this example on a study of an approach mentioned in

Table 6

Test case where *B* is the large CSTR and *A* is a scenario having two small CSTRs (intensified). Values extracted from [10,30]. The value reported in the reference for temperature is given in $^{\circ}$ F, but as we are dealing with incremental values of temperature, we do not need to convert the units to an absolute scale, as discussed in Section 2.1.

Factor	В	Α	d	Fraction	IF _{total}
Volume [m ³]	122	28	1	$(122/28)^1 = 4.36$	0.52
Temperature deviation [°F]	0.4	3.6	1	$(0.4/3.6)^1 = 0.11$	

Section 1, focused on the reduction of process inventory [4]. The process intensification approach considers the minimisation of the inventory for a given production, while classical superstructure optimisations consider usually profit maximisation, or total cost minimisation. It can be argued that such statement is true in a rather literal (strict) sense. Indeed, many superstructure optimisations do focus on cost minimisation; however in practice, the optimisation format easily allows for the replacement of one optimisation criterion by another one. Furthermore, having inequality constraints gives more flexibility in the problem formulation, such that is possible to add a larger number of constraints. For example, an upper bound on the inventory of a component in the process; which can be gradually lowered, and the optimiser can then start searching for intensified solutions.

The authors studied the reduction of ethanol inventory for two weeks in an existing process for producing acetaldehyde via ethanol oxidation, while holding the same throughput of acetaldehyde. In the process, ethanol feedstock is vaporised, mixed with air and fed to a catalytic reactor. The reactor product is scrubbed first with cold dilute solvent (mostly ethanol) and the bottoms of the scrubber are distilled in a first distillation column to recover acetaldehyde as distillate (see Fig. 7). In a second distillation column, organic wastes are collected from the top, and the bottoms are fed to a third distillation column where ethanol (with some water) is separated as the overhead product to be used as fuel in a boiler. The key decision variables in the optimisation problem were the flow rates of ethanol as feedstock and solvent, reaction temperature, the reflux ratio of the third distillation column (to control losses of ethanol) and the reboiler heat load in the first distillation column (to control acetaldehyde recovery). The minimum ethanol inventory for two weeks was 7099 tons at a process yield of 0.315. Approximately 37% less the amount of ethanol stored for the base case (11,239 tons) was found. Also, the option of replacing the reactor and the third distillation column, while simultaneously intensifying the whole process, was also considered by the authors. The results indicate that the addition of new units did provide the same reduction of ethanol inventory than without adding new units.

We select the key variables to illustrate how to apply our methodology (Table 7). The exponent d of the reflux ratio factor was chosen 1 as the energy consumption of a distillation column increases with the reflux ratio. The base solution 1 is compared with a minimum inventory (no new units) case 2, and minimum inventory (with new units) case 3. The calculated *IF* values show how superior the case 3 is compared to 2, which would be hard to spot when only focusing on changing the existing case with 2 or 3 alone. We have opted for not comparing 1 vs 3 since $F_{1-3} = F_{1-2} \cdot F_{2-3}$ (as we did in Table 5, and explained in Section 3.3).

3.6. Internal heat integration in different designs of a propylene splitter

Our last example is based on a Heat Integrated Distillation Column (HIDiC) seen as a energy-conserving unit [31]. The HIDiC combines advantages of direct vapour recompression and diabatic operation at half of the normal column height. With such column the consumption of exergy at approximately the same capital cost is reduced by half with a very short pay-off time, compared to the usual vapour recompression scheme (a column in close boiling mixture separation, see Fig. 8). A comparison of utilities consumption of four different designs of the base case propylene splitter is provided there, of which we select two HiDC cases to compare the 18/13 bar and 18/15 bar pressure setup of the rectification/stripping section (1 vs 2). It is reported that less consumption of the exergy of the conventional vapour recompression system is achieved for the HIDiC with larger stripping section pressure. This is due to the change in the utility consumption from the 18/13 bar case (0.2 kton/year steam and 3358 MWh/year electricity) to the 18/ 15 bar case (1.1 kton/year steam and 1904 MWh/year electricity). The required heat transfer area is the external surface area of the shell of the rectification section column. The increase in column weight is a result

Fig. 7. Schematic representation of acetaldehyde process for which a reduction of process inventory was the goal [4].



Table 7

Test cases where a base solution 1 is compared no new units 2, and with new units 3 (values extracted from [4]).

Case	Factor	В	Α	d	Fraction	IF_{total}
1 vs 2	Reaction temperature [K]	600	580	1	$(600/580)^1 = 1.03$	
	Reflux ratio [-]	3.5	5	1	$(3.5/5)^1 = 0.7$	
	Ethanol inventory	11,240	7100	1	(11,240/	
	[tons]				$(7100)^1 = 1.58$	
	Heat flowrate	0.62	0.76	1	$(0.62/0.76)^1 = 0.82$	
	[MW]					
	Process yield [%]	59	32	-1	$(59/32)^{-1} = 0.54$	0.51
2 vs 3	Reaction temperature [K]	580	610	1	$(580/610)^1 = 0.95$	
	Reflux ratio [-]	5	3	1	$(5/3)^1 = 1.67$	
	Ethanol inventory	7100	7080	1	(7100/	
	[tons]				$(7080)^1 = 1.00$	
	Heat flowrate	0.76	0.76	1	$(0.76/0.76)^1 = 1$	
	[MW]					
	Process yield [%]	32	65	-1	$(32/0.65)^{-1} = 2.03$	3.21

of the need to increase the heat transfer area between the stripping and rectification sections to compensate for a smaller temperature gradient between those sections. This is due to the larger operation pressure in the rectification section in the 18/15 case.

In this case we will highlight a powerful feature of our method, in which we have broken the total number of factors to intensify in three sub-analyses. In the first one, the factors are column height, diameter, weight and bed volume (see Table 8), with which we calculate $IF_a = 0.71$. The $IF_b = 1.43$ is calculated from the transfer area, the tube diameter and pitch. Notice that if we would only have access to this information, we would select the 18/15 bar as the best alternative $(IF_a \cdot IF_b = 1.02)$. When we include in our comparison the utilities consumption of these two designs (last section of Table 8) $IF_c = 1.78$, changing the 18/13 bar by the 18/15 bar has а $IF_{total} = IF_a \cdot IF_b \cdot IF_c = 1.81$ bigger than one, meaning the overall change of equipment is desirable.

3.7. Biodiesel production by integrated reactive separation technologies

This example compares two intensification options, catalytic reactive distillation and absorption, for the production of biodiesel (fatty acid methyl esters, FAME) by esterification of waste oils with high free fatty acids (FFA) content [32]. The esterification of FFA with methanol produces FAME and water as by-product. This reaction is reversible, meaning that by using reactive separation technologies, water can be removed from the reaction medium as the reaction proceeds, allowing for the complete conversion of FFA, while obtaining high purity FAME with a single process unit. In the process based on catalytic reactive

Fig. 8. Schematics of: (a) a conventional distillation column, (b) a column with vapour recompression system and (c) an HIDiC [31].



Test case HIDiC (18/13 bar) compared with HIDiC (18/15 bar); values extracted from [31].

Factor	18/13 bar	18/15 bar	d	Fraction	IF
Column height [m]	66	66	1	$(66/66)^1 = 1$	
Column diameter [m]	2.15	2.15	1	$(2.15/2.15)^1 = 1$	
Column weight [kg]	1.1E5	1.6E5	1	$(1.1E5/1.6E5)^1 = 0.69$	
Bed volume [m ³]	224	217	1	$(224/217)^1 = 1.03$	$IF_a = 0.71$
Transfer area [m ²]	399	779	1	$(399/779)^1 = 0.51$	
Tube diameter [m]	0.7	0.4	1	$(0.7/0.4)^1 = 1.75$	
Pitch [m]	0.8	0.5	1	$(0.8/0.5)^1 = 1.6$	$IF_b = 1.43$
Utility costs [Euros/year]	230,644	142,122	1	$(230,644/142,122)^1 = 1.78$	$IF_c = 1.78$
					$\mathit{IF}_{total} = \mathit{IF}_a \cdot \mathit{IF}_b \cdot \mathit{IF}_c = 1.81$



Fig. 9. Processes for synthesis of FAME by catalytic reactive distillation (top) or catalytic reactive absorption (bottom) [32].

distillation (Fig. 9, top) methanol and FFA are fed to the reaction zone of the distillation column loaded with a solid acid catalyst. Methanol is consumed in the reaction zone, and as a consequence, a mixture of acid and water is easily separated at the top. After decanting, the acid rich phase is refluxed to the column, while water is obtained as distillate. High purity FAME is obtained from the bottom stream after removing methanol by additional flash. Since the reactive distillation column employs extremely low reflux, it behaves rather as a reactive absorption unit, and not as a real reactive distillation unit [32]. Therefore, in the process based on catalytic reactive absorption (Fig. 9, bottom) no products are recycled to the column in the form or reflux or boil-up vapours.

Table 9 shows key variables for the comparison between reactiveabsorption versus reactive-distillation processes [32]. We use these variables to study three intensification factors: the investment cost of the column, the overall cost of the heat exchangers and the operating costs.

We define the intensification factor of the column as the ratio of

column shell investment costs. The cost of a column shell depends on its weight, with a scale exponent around 0.85 [33]. If we assume that the same thickness and material of the column will be used for the reactive absorption and distillation processes, the intensification factor is proportional to the ratio of column volumes (see Table 10). For the sake of simplicity we neglect the cost of column internals. The calculated column IF is 0.85, which indicates that the column for the reactive distillation case will be around 15% cheaper.

Now we discuss the intensification factor of the investment cost of heat exchangers. Since we have limited access to detailed information on the heat exchangers, a simplified comparison is made between the overall costs of the heat exchangers of both processes. We have made the following assumptions: (i) all heat exchangers are of the same type and material, and (ii) the global heat transfer coefficients and temperature differences in all heat exchangers are similar for both processes. With these assumptions, and considering that the cost of a heat exchanger is usually proportional to his area (A) at power of 0.6, the ratio of the overall cost of heat exchangers between reactive distillation

Comparison between reactive-absorption versus reactive-distillation processes at a plant capacity of 10 ktpy (1250 kg/h) fatty esters. The same amount of FFA and methanol are fed to both processes.

	Reactive distillation	Reactive absorption
Column		
Number of stages	15	15
HETP [m]	0.5	0.6
Column diameter [m]	0.4	0.4
Heat exchangers [kW]		
Fatty acid heaters (FEHE1; HEX-1)	95	81; 27
Methanol heater (FEHE2)	8	65
Biodiesel cooler (COOLER)	38	14
Reboiler duty	136	0
Condenser/decanter duty	72	77
Energy		
Steam consumption [kg steam/t FAME]	168	34

Table 10

Calculation of intensification factor reactive-absorption versus reactive-distillation processes [32].

Factor	В	Α	d	Fraction	IF _{total}
Column volume [m ³]	0.94	1.13	0.85	(0.94/ 1.13) ^{0.85} = 0.85	
Weighted Heat Load [kW ^{0.6}]	59.8	51.8	1	$(59.8/51.8)^1 = 1.15$	
Steam consumption [kg steam/t FAME]	168	34	1	$(168/34)^1 = 4.94$	4.83

and reactive absorption based processes, that is, the heat exchanger intensification factor, can be calculated as follows:

$$IF_{hex} = \frac{\sum_{i}^{RD} Q_{i}^{0.6}}{\sum_{i}^{RA} Q_{i}^{0.6}} = \frac{59.8}{51.8} = 1.15$$
(5)

where Q_i is the heat load of each heat exchanger for the corresponding process (RD: reactive Distillation; RA: Reactive Absorption). This approximated calculation indicates that the overall cost of the heat exchangers is similar for both processes. Finally, we note that the operating costs are dominated by the use of steam as utility, and as such, the intensification factor for operating costs is the ratio between steam consumption $IF_{steam} = 168/34 = 4.9$. Therefore, the reactive absorption process seems to be more profitable, because the operating costs are much lower, given that the difference in investment costs between both processes seems to be small. Furthermore, as the reactive absorption based process saves a large amount of steam, this also means a relevant saving in CO2 emissions in a same proportion as IFsteam (assuming that steam is produced on-site by burning fossil fuels). In conclusion, the reactive absorption based process is more profitable and sustainable, which is reflected in a overall intensification factor larger than one.

Table 11

Calculation of intensification factor for traditional water purification versus One-Step Reverse Osmosis.

Factor	В	Α	d	Fraction	IFtotal
Column volume [m ³]	0.94	1.13	0.85	$(0.94/1.13)^{0.85} = 0.85$	
Weighted heat load [kW ^{0.6}]	59.8	51.8	1	$(59.8/51.8)^1 = 1.15$	
Steam consumption [kg steam/t FAME]	168	34	1	$(168/34)^1 = 4.94$	4.83

3.8. Water purification

Here we provide another real-life case, kindly provided by Oasen (The Netherlands), a water utility company that uses sand filters, aeration, active carbon and UV disinfection for the production of drinking water using infiltrated surface water (river bank filtration) as source. The traditional process (Fig. 10a) begins by obtaining filtrated water from the river bank (groundwater), followed by one aeration step, a sand filter step, softening, another aeration and sand filter steps, passage through an active carbon filter, and a final ultraviolet disinfection step that renders the water drinkable.

Reverse osmosis (RO) processes are often used in water treatment trains and facilitate the reusage of high quality water from treated effluent for potable purposes. This is done because it has high removal efficiencies for salinity, inorganic and organic contaminants; it additionally provides an excellent barrier for pathogens [34]. Oasen is implementing a novel process intensification called One-Step Reverse Osmosis (OSRO), see Fig. 10b. This concept begins also with river bank filtrated water, followed by a Reverse Osmosis step, passage through an Ion Exchange membrane for the removal of NH_4^+ , a remineralisation step where Ca²⁺ is added and pH is corrected, finalised with an aeration step that makes the water potable. There is a significant reduction in the number of process steps of the new this OSRO concept (4), in contrast to the traditional scheme (7). The production capacity of this concept is expected to be 3.5 million m³ drinking water per year. The parameters selected to evaluate the method presented in this paper can be seen in Table 11. The selection was made by the project department of Oasen, since they have all the knowledge about engineering and building plants. Based on the calculated IFtotal value (18.56), OSRO should be a better alternative to the current technology, which is the same outcome found by the company when a business case was made for the newly planned production plant (and before knowing about the method proposed in this work).

The log removal value (LRV) is a very strong indicator for the removal efficiency of a particular component (chemical or bacteriological). The higher the LRV, the higher the drinking water quality, e.g. 1 LRV = 90% reduction of the target component, 2 LRV = 99% reduction, and so on) [34,35]. Note that we have included in our analysis a factor of relevance, not only for the company, but also for the environment: sustainability. The sustainability factor is based on a





Fig. 10. (a) Traditional water treatment train with seven steps (filtration, aeration, sand filtration, softening, second aeration, second sand filter step, active carbon filter, and a final ultraviolet disinfection step. (b) Novel process intensification called One-Step Reverse Osmosis (OSRO) with only four steps. qualitative decision, which means there are no "hard figures", and it is just an overall impression of the sustainability OASEN's team opinion. For example, they are not using CO_2 equivalents, which is less sustainable-oriented. The "+" symbol means that there is a positive perception; similarly, "+ + +" is a subjective assessment in which the process is assigned a numeral accordingly: + + + = 3.

4. Discussion

Here we provide a general discussion relevant for all cases analysed before. The first one we have identified is that there might be risks of considering a given factor or weight more than once. This could happen based on different terminologies used by experts in different activities or historical documents. Additionally, depending on how the information or "factors" are calculated, some hidden elements could inadvertently be left out. As a compensation, besides the obvious benefit achieved after normalisation of values by dividing each IF, the only action to reduce this possibility is to have a transparent database and ask for external auditing of the method.

Taking as an example the OBR case (Section 3.1), Pressure is a factor that could be considered important to "decrease" in one analysis, but the opposite could also happen. For this we think is useful to define two times an *IF* having both alternatives:

- 1. When lower pressure is desired for safety reasons, d = 1.
- 2. When the increase is needed for improved kinetics, d = -1.

Alternative 1 would have an $IF_{total} = 1195$ as calculated in Section 3.1, whereas the new $IF_{total} = 3443$ of Alternative 2 would indicate a stronger argument to replace the existing equipment. Here the role of the analysts or experts comes as the most important decision step, deciding whether Safety is more "desired" or the improved kinetics alternative. If the experts would decide to include both alternatives for a more inclusive analysis, a new Intensification Factor could be calculated having different *d* values.

As mentioned in Section 2.1, the choice of scales used for each F when calculating the *IF* value needs to follow some basic guidelines, such that it is invariant to a change of the physical scale in any of the performance factors F_i . If two intensification teams in two different locations (say Europe and North America) are working on a same problem, there needs to be an agreement on which scale to use, for example in the case of temperature (Fahrenheit or Celsius). To avoid these situations, it is necessary to use scales that have an absolute zero in a physical sense.

The final discussion we want to emphasise is the last case (Section 3.6) where the importance of having all available information for a given analysis is evidenced. For the case of a total value $IF_{total} = IF_a \cdot IF_b \cdot IF_c$, having only the values corresponding to alternatives *a* and *b* would motivate the change of the second option. If the decision would have been based on the technical experts alone, the result would certainly be different to the situation in which the economical aspects *c* are included.

5. Conclusions

We believe to have given sufficient evidence of the advantages of using a simple evaluation tool, based on a method for intensification factors calculation. Together with a step-by-step procedure, and examples extracted from scientific literature, as well as from industrial practice, we think the reader can start applying this tool to his own problems (academic or industrial). This method has been employed in pedagogical settings while teaching a Process Intensification Principles course at the University of Twente. The students have managed to understand better the advantages of intensifying a given process by making use of this simple method.

Another important argument is that this method might seem

superfluous to experts who have worked for many years in intensification or innovation of chemical processes. However, for outsiders or non-experts on a particular process to be improved, we believe our proposed method comprises very simple mathematic operations that can be understood by most educated persons without a specialisation in chemical engineering. For example, in companies such as small and medium enterprises, spin-offs or other multidisciplinary settings, normally there is only one expert; convincing other non experts from marketing, finances, etc., is a challenge we have aimed at resolving with this method.

Our simple method rests on the value assignment of two exponents: c_i and d_i . The first leads to a "base case" at the beginning of a project, when all $c_i = 1$, and such IF_{total} value can be used as a benchmark for improvements in advanced phases of the specific project. The d_i allows to express when the increase or decrease of a given factor is desired or not.

More limitations besides those hinted in this work will be found as the method is tested in real life scenarios. Identifying the weak aspects and improving them, such as increasing the analytical power (weights determination, etc.), will be more efficient as other colleagues use it and their findings are reported. Practice will tell if this simple method is of use beyond what the authors have already identified and reported here. We are aware that it has already been used by a spin-off company, BuBclean, VOF, The Netherlands, to report to their clients and in subsidies proposals. Similarly, OASEN BV, The Netherlands, has used the method and compared the result of using this method with an existing business case employed for the decision of building a new plant.

As a follow-up for this paper, we have created a group in "LinkedIn" as a means to open a discussion where academic and industrial scientists share their experiences in using this method. The title of the group is Intensification Factor initiative, its weblink can be found in the link https://www.linkedin.com/groups/7062911. We expect experts from different communities to share their ideas and experiences to test the validity of this method.

Conflict of interest

DFR is co-founder of BuBclean, and has no financial interest in it; WvdM is CEO of OASEN, and no conflict of interest has been identified.

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