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Sustainable Process Systems Engineering for Chemicals within Planetary Boundaries

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ABSTRACT

The planetary boundaries (PBs) define ecological limits that are critical to preserve the stability of the Earth. Six of them have already been exceeded, which calls for urgent action to optimize industrial systems capable of operating within the safe operating space that they define for humanity. Here we discuss the challenges and opportunities of including PBs in a range of application domains in Process Systems Engineering, focusing on chemicals and fuels production and the use of mathematical programming coupled with life cycle assessment to support sustainable decision-making.

Keywords: Environment, Renewable and Sustainable Energy

INTRODUCTION

The role of the planetary boundaries in the transition to sustainable chemicals

The chemical sector currently faces the challenge of curbing its carbon emissions to meet the climate goals. This will require replacing fossil carbon with renewable carbon as main feedstock, either in the form of captured CO_2 from the air, waste (e.g., polymer waste) or biomass. Unfortunately, emerging renewable-carbon based technologies often lead to inherent trade-offs when compared to the fossil business-as-usual counterpart, not only in terms of cost vs. environmental impacts, but also between environmental categories. For example, chemicals produced *via* carbon capture and utilization (CCU) are often expensive due to the high cost of electrolytic hydrogen, while at the same time could worsen human toxicity impacts owing to the large amounts of renewable power required to activate the CO_2 molecule [1].

This occurrence of burden-shifting (one impact, e.g., global warming, improves at the expense of worsening others) should be carefully investigated to ensure a truly sustainable transition to a defossilized chemical sector. However, while the environmental assessment methods that exist today are useful for comparing alternative technologies, they provide very limited insights into their impact in absolute terms. Because of this, the broad implications of the large-scale deployment of technologies, specifically concerning their potential global environmental collateral damage, remain unclear, which can lead to spurious conclusions and wrong advice.

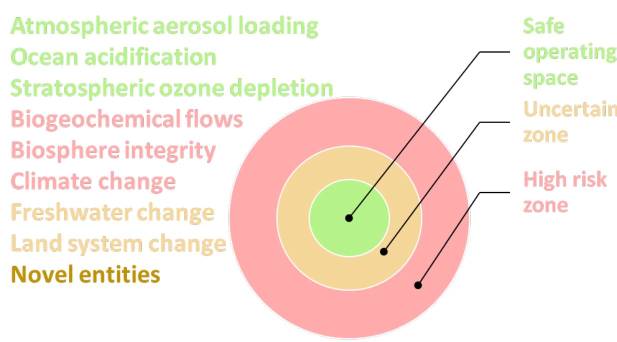

Figure 1. Planetary boundaries defined on nine Earth-system processes. Earth-system processes are coloured according to the current trangression level (note that the upper end of the zone of increasing risk has not yet been quantitatively defined for the novel entities PB [3]).

The planetary boundaries (PBs) provide an excellent framework to evaluate the global damage on the planet of emerging routes and the severity of burden-shifting when attempting to combat climate change. The PBs, originally proposed by Rockström et al. [2], define limits on nine Earth-system processes (Fig. 1), all key for regulating the stability of the planet. For each Earth-system process, thresholds were proposed that define a safe operating space (SOS) for humanity for many centuries to come. Exceeding such limits could trigger critical events that could challenge the resilience of the planet and shift its equilibrium state to a new one with unknown consequences. According to the latest update, six PBs (out of nine) have been already transgressed [3], which calls for urgent action to design and operate chemical systems within the ecological limits of the Earth.

The PBs were not originally intended to be directly applied to industrial systems, yet recent work linking emissions data to impacts on the PBs control variables enabled their application to chemical processes. Standard life cycle assessments (LCAs), the current prevalent approach to evaluate chemical technologies environmentally, lack absolute thresholds to interpret impact values. This shortcoming limits their application to relative comparisons, as already said. Specifically, given two alternative technologies, we could conclude with a standard LCA that one is less environmentally impactful than the other in a given category, but whether they are truly sustainable in absolute terms would remain unclear. The PBs explicitly address this specific question by comparing impact values with a given threshold derived from the carrying capacity of the planet Earth (Fig. 2). If the threshold is exceeded, the system is deemed unsustainable, and would be considered sustainable otherwise. Hence, coupling LCA with PBs allows to explicitly evaluate whether industrial systems operate sustainably within the Earth's ecological capacity.

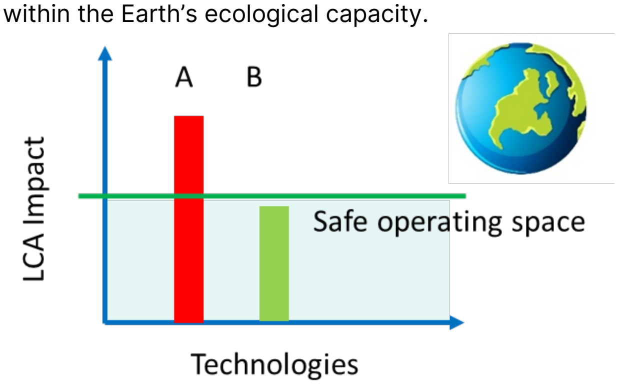

Figure 2. Application of PBs to the assessment of industrial systems. A threshold based on the PBs is established to interpret the impact values quantified *via* LCA.

PLANETARY BOUNDARIES IN PROCESS SYSTEMS ENGINEERING (PSE)

Planetary boundaries application to industrial systems

The PBs assessment of technologies comprises two steps (Fig. 3). First, a share of the SOS is assigned to the system studied following some downscaling (sharing) principles. The SOS should be shared among all economic activities jointly, so shares of the total budget need to be defined and allocated to the specific system investigated prior to the assessment. This is a controversial step on which there is no consensus yet and that can result in different environmental budgets depending on the principle applied. Once the threshold is established for a given chemical system, a standard LCA is conducted. However, in the impact phase, impacts on the control variables of the PBs (rather than standard LCIA metrics) are determined using recently developed planetary damage models [4-5]. In the last LCA step, the results are interpreted, and conclusions and recommendations are provided considering the planet-wide impact of the studied industrial system.

The added value of performing an absolute LCA based on the PBs is that it allows classifying systems as sustainable or unsustainable in each Earth-system process. This, in turn, allows interpreting environmental trade-offs by quantifying the extent to which processes contribute to trespassing global boundaries, noy only those linked to climate change.

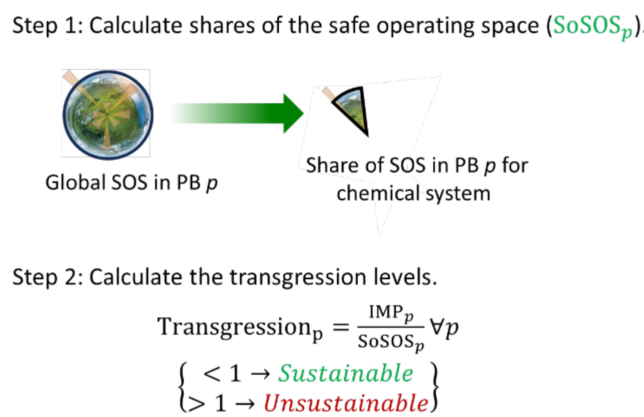

Figure 3. Application of PBs to the assessment of industrial systems. First, a share of the SOS is determined. Then, the transgression level is calculated by comparing the impact values with such a share.

PBs were originally defined to monitor the environmental state of the planet Earth. Here I argue that they could also be incorporated into the design and operation of sustainable industrial systems as additional constraints/criteria, to enforce that they ultimately comply with global environmental guardrails that are essential for ensuring sustainable development. This paradigm shift towards PBs-based decision-making opens the door for a myriad of applications, within the chemical sector and beyond, for which computer-aided tools quantifying explicitly the PBs impact of engineering decisions across scales could be developed. While, in principle, any industrial process could be evaluated using the PBs, PBs studies are (arguably) better suited to large-scale systems with large potential impacts that could destabilize Earth-system processes. For example, PBs assessments of bulk chemicals, such as ammonia, might be more relevant as their current fossil production routes emit large amounts of CO_2 contributing strongly to the transgression of the climate change boundary, regarded as a core planetary boundary. On the other hand, PBs assessments of chemicals produced at smaller scales might be less appealing, as the implications for the planet's stability will likely be less critical. Note, however, that the control variable for the novel entities PB is, in principle, independent of the quantities produced (i.e., percentage of synthetics released into the Earth system) [3], so the above might not hold fully true for this case.

Overall, the PBs framework provides valuable insights out of reach for standard LCAs, and here I suggest that they are adopted in sustainability problems to complement other environmental metrics, ultimately guiding research and policymaking more sensibly.

Application domains in Process Systems Engineering

The PBs offer a comprehensive framework to design sustainable chemical systems operating within the SOS. In essence, this could be accomplished by leveraging the existing life cycle optimization framework [6], widely applied in PSE [1, 7-8], in conjunction with the recently proposed PBs characterization factors [4-5]. Following the life cycle PBs-based optimization approach, an optimization model shall be formulated where life cycle assessment principles are explicitly included *via* linear constraints linking mass and energy flows with emissions data and their PBs impact, as shown in the general compact formulation below.

$$\begin{aligned} \min \quad & f(x,y) \\ s.t. \quad & h(x,y) = 0 \\ & g(x,y) \leq 0 \\ & \sum_i CF_{ip} LCI_i \leq SoSOS_p \quad \forall p \\ & x \in \Re^n, y \in \{0,1\}^m \end{aligned}$$

Here, $f(x,y)$ represents the objective function to be optimized, often related to economic performance, whose value is determined from the continuous variables x (e.g., temperatures, pressures, capacities of supply chain (SC) nodes, etc.), and binary variables y (e.g., selection of unit operations in a process flowsheet or SC entities in a network problem). Equality and inequality constraints describe the system studied and may include, in addition to the formulas required to compute the objective function value, equations linked to mass and energy balances and thermodynamic constraints in process synthesis problems, or capacity limitations and mass balances in supply chain problems. An inequality constraint can be added to the model to impose a maximum impact on the PBs. To this end, we link the life cycle inventories entries *i* (i.e., life cycle feedstock requirements, emissions and waste calculated for the functional unit taken as a basis in the LCA calculations) to the impact on the control variables of the PBs using tailored characterization factors CF_{ip} defined for each Earth-system process *p*; moreover, we enforce that the resulting impact should not surpass the share of the SOS allocated to that particular system. Such a PBs constraint might be relaxed, allowing the system to transgress the PBs share, while penalizing such transgression in the objective function using slack variables and penalty coefficients.

The optimization model can take distinct forms depending on the scope of the analysis, e.g., MILP/LP in sectoral and supply chain problems or an MINLP in process synthesis or molecular design problems. We can then capitalize on the rich optimization theory and existing software tools to identify solutions with minimum PBs impact (for further details on mathematical programming applied to sustainable process systems engineering, see [9-12]) Moreover, standard LCAs, extensively employed in the environmental assessments of a wide range of chemical technologies, can be easily enlarged in scope to evaluate the PBs impact, thereby providing additional insights. These conventional LCAs have become very popular in chemical engineering, with increasing applications in the evaluation of low TRL chemical technologies [13].

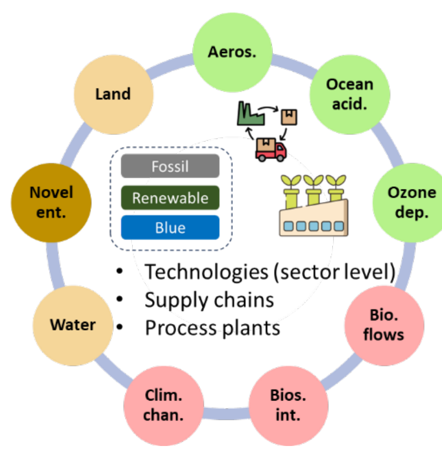

Figure 4. Examples of application domains across scales, including network models optimization (at the sector level), supply chain optimization, and process design.

Focusing on PSE application domains (Fig. 4), the areas of sectoral analysis (network modeling), supply chain optimization and process synthesis seem to offer the largest potential for applying the PBs framework. In network models, a superstructure of technologies is postulated to find the best portfolio to cover the demand of given products, often at minimum cost. Superstructures were for example defined for biomass routes to chemicals and fuels [14], CCU technologies [1] and chemical recycling pathways [15]. Here the problem is often formulated as an LP, using simplified equations based on linear yields to model technologies. Such simplified network models are typically employed to generate insights into the best routes to meet some demand (top-down) or the best technologies to transform given feedstock into valuable products (bottom-up). The spatial scope can be quite broad, particularly when considering global demands and capacity limitations based on the global availability of resources. Network models are very well suited to identify technologies that are truly sustainable in absolute terms. Here, a share of the global SOS can be allocated to the demanded products to define environmental constraints that should not be violated, as we did in recent work where we studied how to produce plastics sustainably within the PBs [16].

At a higher level of detail, supply chain (SC) models optimize the network topology and associated operations, including the location and capacities of nodes (e.g., plants, warehouses, distribution centers) and the production rates and transport flows between the SC entities. The inclusion of PBs in standard SC formulations is of particular relevance when considering technological decisions, which often lead to critical trade-offs. For example, we recently included PBs in the optimal design of hydrogen supply chains, finding solutions that decrease substantially the pressure exerted on the Earth-system processes by replacing grey with green H_2 [17].

PBs could also be considered in process design problems to find the optimal topology and operating conditions to optimize economic performance while respecting global environmental limits. One option here is to formulate the design problem in global terms, focusing on finding the optimal design of a plant of standard size that could be installed across the world to cover the global demand of given chemicals. Because the technology (chemical pathway) is already fixed here, the potential for environmental gains is typically more modest. This is because once a chemical route is selected, processes implementing such a pathway often operate near the stoichiometric amounts of the required reactants, which often constitute the main environmental hotspot contributing the most to total impacts. Notably, although heat integration can still play a role, impacts (particularly in bulk chemicals) are sill mostly dictated by the raw materials' environmental footprint. Consequently, implementing alternative unit operations and optimized operating conditions is unlikely to reduce the impact sharply unless the provenance of the reactants is modified (e.g., grey vs. green H_2 in carbon capture and utilization routes). However, given the large production volumes of some chemicals, particularly bulk chemicals, even marginal improvements are worthy to pursue. Recently, we introduced PBs in the design of a methanol flowsheet, letting the model select the hydrogen source depending on the objective function optimized. We found that substantial reductions in global impacts can be attained by resorting to renewable carbon feedstock [18].

Lastly, PBs can also be easily incorporated into standard LCAs. For example, using absolute sustainability LCAs based on the PBs, we showed that almost all widespread fossil chemicals transgress at least one PB due to their large CO_2 emissions [19]. We also demonstrated with LCAs based on PBs that current fossil platform chemicals require around one quarter of a planet to operate, also owing to their large carbon footprint, and investigated ways to defossilize chemicals production sustainably by shifting to renewable carbon sources [5].

CONCLUDING REMARKS

The chemical sector should transition to defossilized technologies to close the carbon loop and operate sustainably within the Earth's ecological capacity. This will require assessing and minimizing the unintended detrimental effects of emerging routes on environmental categories beyond climate change. In this context, the planetary boundaries offer an excellent framework to perform holistic assessments and identify solutions operating within the safe operating spare for humanity. Here I argue that due to its systems thinking and powerful computer-aided tools, Process Systems Engineering is in a unique position to embrace this new methodology in current assessments and optimizations of sustainable industrial systems, from molecules, through process to supply chains, sectors and the planet level.

By incorporating the impact on the PBs explicitly in decision-support tools, the broad environmental implications of chemical systems will become clearer. This will allow us to identify the most promising technologies consistent with the planet's ecological capacity early on, guiding experimental research and policy-making more effectively.

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