Abstract

While several engineering and science disciplines, including biology and environmental science, have greatly benefited from adopting a systems thinking approach, its extension to chemistry education is a much more recent advancement. The initial body of literature in this direction has largely surveyed the feasibility for systems thinking in general chemistry courses. Herein, we go a step further to explore the possibilities that systems thinking presents for the instruction of more advanced chemistry courses, specifically in the context of catalysis education. Since catalysis has conventionally been taught employing a reductionist perspective, we identify the opportunities and challenges for instructors in transitioning to a systems thinking teaching style. We build our analysis in accordance with the principle of constructive alignment, where we systematically address the implications for systems thinking in writing intended learning outcomes, designing learning activities and formulating student assessments. Through a series of carefully crafted examples in homogeneous as well as heterogeneous catalysis, we illustrate how embracing systems thinking can potentially enable a paradigm shift in catalysis education.
Introduction

Systems thinking (ST) is defined as an approach to examine complex behaviors and phenomena from a holistic perspective. This is in contrast to a reductionist approach, wherein one tries to understand a phenomenon through the analysis of its constituent components. The reductionist viewpoint has enriched fundamental molecular-level understanding in chemistry. It has also greatly aided in the advancement of knowledge across different science disciplines, but there is increasing evidence to suggest that this perspective must be complemented with a ST approach to address impending issues and pressing questions in the future.

Several definitions of ‘system’ and ‘systems thinking’ have been postulated over the years. The three essential characteristics of a ‘system’ are (i) there are multiple elements or components, (ii) they have interconnections, and (iii) there is an overall purpose. A thinking approach that (i) recognizes the system as a whole and not merely as a collection of parts, (ii) examines relationships between parts of a system, (iii) identifies factors that cause system-level emergent behaviors, (iv) examines the evolution of system properties over time, and (v) identifies the interactions between a system and its environment, constitutes ‘systems thinking’. With respect to the final point, the term ‘boundary’ is used for what separates the system from its environment.

Two important branches of science, namely biology and environmental science, have made significant strides after espousing a systems approach. In environmental science for instance, a cradle-to-grave holistic approach is at the heart of life-cycle assessment. Despite allied disciplines reaping great benefits by virtue of adopting a systems approach, chemistry has remained largely reluctant to embrace this perspective. It was only in 2017 that a dedicated IUPAC project was started for this purpose. The December 2019 special edition of the Journal of Chemical Education presented the outputs of the project, where the importance of extending ST to general chemistry education was emphasized through multiple articles. Other articles published elsewhere in the recent past identified general chemistry courses as being predominantly formulated with a reductionist outlook, wherein concepts and applications are taught in a disjointed and fragmented manner. A similar approach is also applied to conventional advanced chemistry courses ranging from organic and analytical chemistry to catalysis. Reorienting the way chemistry courses are taught to espouse ST will enable instructors to better illustrate the interconnections between core chemistry concepts and the larger earth and societal systems. This can significantly transform the way young learners perceive topics like green and sustainable chemistry. This is one branch of chemistry where ST is relatively easier to establish because the interdependencies between the chemical processes subsystem and the environmental factors subsystem is the pith of the topic.
Effective communication of sustainable chemistry will have a direct bearing on how next-generation chemists work towards the attainment of globally important targets, such as the United Nations Sustainable Development Goals.\textsuperscript{27-28}

The objective of this article is to identify opportunities to promote a ST learning approach in a catalysis course. This is different from the vast majority of published literature, which focusses on lending a ST perspective to general chemistry courses typically taught in the first years of the undergraduate curriculum. The challenges to promote ST in a specialized course, such as one on catalysis, are different. Course modules based on catalysis are usually delivered to students in the second half of their undergraduate studies, with more advanced course units often being taught at the M.Sc. level. At these levels, students are mature enough to realize that chemistry concepts and environmental subsystems are not two entirely disconnected worlds. As a subject, catalysis is highly contextualized too. However, ST competencies go much beyond the acknowledgement of environmental implications and an ability to understand context. In addition to this, catalysis is inherently a ‘zoomed in’ topic, dealing with aspects, such as studying the active site, reaction kinetics and catalyst synthesis. Yet employing only a reductionist didactic approach has been found to inculcate fragmented and siloed knowledge in students.\textsuperscript{21, 29} Hence, the challenges in (re)designing a catalysis course that strives to activate ST are manifold. Foremost of the challenges is to marry a ‘zoom out’ perspective to the implicit ‘zoomed in’ nature of the subject. Secondly, students will be introduced to several catalytic processes and reaction mechanisms during the course. All of this knowledge must not be relayed as piecemeal presentations of information, but through ST, students must be able to identify the overarching chemistry and catalysis concepts. Furthermore, the emphasis would need to shift from ‘applying a concept in a particular context’ to ‘applying a concept in different contexts’. Finally, the interface between the environmental subsystem and catalysis concepts needs to be illustrated in a manner that provokes students to place environmental considerations at the forefront of their thinking instead of merely stimulating a cursory acknowledgement of environmental consequences of catalysis-related decisions.

We begin with an analysis of the content that is presented in catalysis courses at universities and covered in many standard textbooks. We survey typical learning objectives in this topic and explore how they would have to be reconsidered to promote ST. The functions and advantages of graphical tools for ST in catalysis education are demonstrated through two examples: one at a broader course-level, and another at a specific concept-level. Subsequently, we move on to highlight learning activities that involve ST. The article concludes with a section addressing ways to assess students’ accomplishment of ST outcomes in catalysis. The intention of this article is to stimulate the catalysis education community by showing the scope for systems thinking in this discipline. Therefore, the aim is not to provide
an exhaustive treatment of ST in catalysis, but to explore the realm of opportunities that a ST approach offers for enhancing the students’ catalysis learning experience.

**Catalysis course content and learning outcomes**

Figure 1 presents a compilation of keywords describing the main sub-topics of interest in a catalysis course module framed in a petrochemical context. A general catalysis course can be divided into two components, namely homogeneous and heterogeneous catalysis. Both these branches require an introduction of fundamentals, including thermodynamics and kinetic principles, and basics of organometallic chemistry. The purpose of the figure is not to present a comprehensive list of the topics that are taught in a catalysis course, but instead is to establish the technical background to which we seek to extend ST in this article. While examples in petrochemical catalysis are cited herein, which admittedly, are fundamentally different to fine chemical synthesis, the incentives of adopting a ST approach hold across contexts. There is often an apprehension in instructors of chemistry courses that the depth of the scientific content to be covered leaves them with little scope to change their pedagogical style significantly, as such a step would reduce the time available for delivering technical content. Bearing this in mind, we try to identify pedagogical opportunities to promote ST across a large board of topics (Figure 1) without diluting the technical rigor, but through a repackaging of existing content that embeds the ST approach.

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**Figure 1. Overview of the most important topics, concepts, and keywords in catalysis education.**
The current style of catalysis education is tailored to provide a context-based learning experience. For instance, in homogeneous catalysis, concepts like the 18-electron rule, oxidative addition, reductive elimination and migrative insertion, are invoked and applied during the instruction of several industrially important reactions, such as carbonylation and hydrogenation (Figure 1). Likewise, the properties of industrial catalysts like zeolites are always elucidated with the help of real-world industrial applications. Hence, the reductionist approach to catalysis instruction cannot be criticized for a lack of context.

When a course outline is formulated without a holistic mindset, the intended learning outcomes (ILOs) end up being largely reductionist, say for example, ‘to describe methods to characterize chemical and physical properties of heterogeneous catalysts’ or ‘to explain the catalytic cycle of important homogeneously catalyzed reactions: hydroformylation and metathesis’. The first ILO does not seek to relate or integrate the ‘catalyst characterization’ subsystem with other subsystems. Even when characterization techniques are taught through concrete applications to industrially used catalyst materials, such a didactic approach is directed at building contextualized but localized knowledge domains. ST aims to go a step further; for example, how does the characterization data relate to the synthesis procedure, which characteristics of the characterization data serve as a fingerprint for catalytic activity, and how do the sample treatment and reaction conditions affect the characterization method and data. For students to be able to explore such questions that are at the interface of subsystems (catalyst synthesis, catalyst characterization and catalytic active site), course ILOs would have to be rewritten. Perhaps, the best starting point for rewriting ILOs is the overarching learning outcomes prescribed by Pazicni and Flynn. For the catalysis discipline, these would translate to: (i) to develop systems thinking skills using catalysis and (ii) to demonstrate catalysis knowledge via systems thinking. Extending from this, an exemplar ILO would be: ‘students will be able to apply systems thinking to catalysis to better understand fundamental catalytic processes and underlying physical and physical chemical mechanisms that leads to the design of better and more sustainable catalysts and catalyst systems.’ Thus, ST-based learning outcomes place core catalysis concepts at the intersection of closely allied subsystems and disciplines, which automatically mandate a holistic thinking approach for their fulfillment. From an instructional standpoint, this places emphasis on choosing the subsystems appropriately, which as discussed in the following section, can be achieved through various graphical tools.

**Graphical tools for ST in catalysis**

*System-oriented concept maps for heterogeneous catalysis*

Systems-oriented concept map extension (SOCME) is an elegant and comprehensive graphical tool to foster ST in chemistry education. A SOCME allows for the identification of subsystems, the interrelationships between them, and the dynamic aspects of the
interdependencies. The subsystems can be chosen to represent learning outcomes of a particular course, but this need not always be the case, which makes SOCMEs a highly flexible tool. Figure 2 shows a SOCME that has been drawn with an objective to set the stage for the heterogeneous catalysis component of the course. The SOCME illustrates the links and dependencies of core heterogeneous catalysis and characterization concepts on the catalytic process as a whole, as well as environmental and economic considerations. The SOCME defines the boundaries of the different subsystems under consideration and illustrates interrelationships within and across boundaries. Along with instilling a ST approach in learners from the very beginning, such a SOCME is also of immense use to an instructor wanting to revamp the course curriculum to incorporate holistic thinking in catalysis. At the outset, the SOCME can also be used to illustrate differences between homogeneous and heterogeneous catalysis. We have identified several nodes across different subsystems, labelled with an asterisk in the SOCME (Figure 2), which can be used as basis to draw comparisons between the two types of catalysis. While not presented here, these common nodes can be used to develop a separate homogeneous catalysis SOCME, similar to the one shown in Figure 2.

Pazicni and Flynn state that “engaging systems thinking skills may help students gain deeper insight into chemistry – in three potential ways”. These are (i) insights into the discipline itself, (ii) insights into how knowledge in the discipline can be used to understand processes in other allied disciplines, and (iii) insights into how the discipline of interest interacts with environmental and economic factors (human experience). The SOCME sketched in Figure 2 harnesses all three insight channels. The ‘core heterogeneous catalysis concepts subsystem’ and ‘core heterogeneous catalyst synthesis & characterization concepts subsystem’ provide insights into the discipline of heterogeneous catalysis. The interactions of these subsystems with the ‘catalytic process subsystem’ illustrate how core concepts of heterogeneous catalysis explain the functioning and design of a catalytic reactor (allied discipline). Likewise, the SOCME shows how the ‘reaction conditions subsystem’ regulates or influences different aspects of the heterogeneous catalytic process. Finally, the ‘environment and economics subsystem’ expresses the interaction of conceptual knowledge domains with human experience factors.

Students are usually introduced to kinetic models like the Langmuir-Hinshelwood model and the Eley-Rideal mechanism through the use of concrete catalytic examples. While these examples provide relatable and comprehensible context to the mathematical expressions of the models, they do not inform the student of the relevance of the models in the larger scheme of things. It is in such instances where a SOCME serves as a very useful tool. Figure 2 illustrates that standard kinetic models describing the intrinsic rate of a catalytic reaction help in formulating the overall rate expression of the reaction, which is an important input for reactor design that calculates the volume of a reactor and weight of catalyst to be used. An efficient
reactor design is key to having an efficient process on the whole, which also relates to environmental and economic factors.

Figure 2. A SOCME for a course unit on heterogeneous catalysis. The SOCME shows the components and interconnections of the following subsystems: catalytic process (yellow), reaction conditions (red), heterogeneous catalysis concepts (blue), heterogeneous catalyst synthesis & characterization concepts (purple), and environment & economics (green). Examples of nodes across different subsystems that can be used to compare and contrast homogeneous and heterogeneous catalysis are marked with an asterisk.

The SOCME also helps students realize system-level properties. For example, the SOCME shows that the rate of a catalytic reaction need not always be the same as the intrinsic rate, but can be significantly altered by physical phenomena like mass transfer and diffusion (Thiele modulus/effectiveness factor branch) and chemical phenomena such as catalyst deactivation. These phenomena often have non-linear effects on the observed rate of reaction and product yield that cannot be described through a linear combination of constituent factors. Furthermore, SOCMEs that include feedback loops help establish cyclic behavior and relationships. Through Figure 2, the student realizes that the use of in situ characterization methods aids in studying and identifying the catalytic active site, and that this information can be used to modify catalyst synthesis protocols to design a catalyst material with a greater number of active sites, which
can again be examined and corroborated through characterization methods. The SOCME drawn in Figure 2 does not include all the heterogeneous catalysis concepts that are typically covered in a course module. The missing components and interactions constitute opportunities for learners to expand on the map further. For instance, aspects of chemoselectivity, undesired waste generation, and more environmental and human health impacts can be embedded into the SOCME during discussion. Thereby, the SOCME doesn’t only serve as an instructional tool but also has an interactive element to it, allowing students to update the figure as the course evolves.

**Process network diagrams in homogeneous catalysis**

In the next example, we explore the use of a graphical tool to foster ST in homogeneous catalysis. Let us consider the Monsanto process for the production of acetic acid, which was one of the first large-scale industrial applications of homogeneous catalysis.\(^{33}\) Catalytic cycles, such as the one in Figure 3 for the Monsanto process are commonplace in homogeneous catalysis education. The scheme depicts important steps of the main catalytic cycle, including oxidative addition, migration, ligand addition, and reductive elimination. However, the myopic nature of the scheme to solely focus on these individual steps of the reaction mechanism does not aid in addressing the Monsanto process holistically. We advocate the use of a more comprehensive ‘process network’ (Figure 4) to supplement the traditionally used catalytic schemes (Figure 3). The green dotted lines in Figure 4 show the chemical transformations that occur as part of the desired catalytic cycle; thus, the main steps of the catalytic cycle drawn in Figure 3 are also incorporated in Figure 4. However, in addition, Figure 4 also highlights the following:

- the undesired reaction between methanol and carbon monoxide yielding methyl formate (red solid line)
- the undesired rhodium-catalyzed water-gas shift reaction yielding hydrogen and carbon dioxide (red dotted lines)
- the water-assisted reductive elimination of CH\(_3\)COI yielding the desired product, acetic acid (green solid lines)

Hence, Figure 4 provides a more complete picture of the Monsanto process, thereby allowing learners to appreciate the relationships between the different components of the system. Such process network schemes can be considered analogous to systemigrams, which generally depict a flow of information from the top left to the lower right, or in other words, show the transformation of an input to an output from left to right.\(^{32}\) Figure 4 is built on a similar template, showing the conversion of reactants stacked on the left to products stacked on the right.
The process network allows recognition of the different reactions that a reactant molecule or catalyst species undergoes. The participation of a molecule/coordination complex in both desired and undesired reaction steps can be discerned by following the connections extending out of the corresponding node. This aids in easier understanding of cause-effect relationships on a systems level. Multiple complementing and contrasting effects may be induced through a change in one component of the system. For instance, water assists the desired reductive elimination of CH$_3$COI (green solid line, Figure 4), but also promotes the undesired water-gas shift reaction (red dotted lines, Figure 4). Thus, the advantages and disadvantages of a high concentration of water in the Monsanto process can be elucidated through a ST lens. Even in the absence of a ST approach, instructors touch upon the deleterious effects of water to motivate the Cativa process (catalyzed by Ir) for the same reaction. Therefore, the same information that is currently used as a 'link' to the next topic can be conveyed in a manner to promote ST. As opposed to promoting siloing of knowledge with very specific links, the remodeled didactic style encourages students to visualize the larger system, understand the interconnections, and realize the motivation for subsequent topics through ST.

The necessity to continue to use traditionally drawn catalytic cycles, as in Figure 3, alongside a wider-ranging process network diagram stems from the limited capacity of the 'working memory'. As per the information processing theory, new information is first transferred to a 'working memory' before becoming part of 'long-term memory'. The all-inclusive nature of the process network scheme (Figure 4) poses a high risk for cognitive overload due to the limited capacity and duration of the working memory. This is why a focused 'zoom-in' approach (Figure 3) must complement the 'zoom-out' systems thinking approach (Figure 4).
Figure 4. A process network diagram of the Monsanto acetic acid process. The starting reactants are in rectangular boxes, catalytic intermediates in ellipses and final products in triangles. The reaction steps of the desired and undesired catalytic cycle are represented using green and red dotted lines respectively.

We also believe that process network diagrams can be extended to discuss the nature of the feedstock (aspects of availability and sustainability) and the environmental impact of the products. Since the reactants and products are stacked on opposite sides, as in Figure 4, it would be easier to add sub-nodes detailing the fossil fuel-based production of CO (on the reactants side) and the environmental implications of CO₂ emissions (on the products side). Likewise, a conversation on the criticality of the elements used here as catalysts (Rh or Ir in Cativa process) in terms of relative abundance, supply risk and environmental implications can also be initiated. By considering such implications, we encourage thinking at a level higher than treating Monsanto process as a standalone acetic acid manufacturing technology. This can be considered analogous to the interaction of the ‘environment and economics subsystem’ with other subsystems depicted in the SOCME for heterogeneous catalysis in Figure 2.

Learning activities for ST in catalysis

The principle of constructive alignment states that the learning experience offered by the teacher must support the learners to achieve the end-goal, or equivalently, the course learning objectives. More specifically, the term ‘constructive alignment’ refers to the alignment of learning activities and assessment tasks to the ILOs. The same principle needs to be followed
to achieve systems thinking in catalysis as a learning outcome. In this section, we discuss the design of learning activities to foster ST in catalysis.

**Think-Pair-Share for ST learning activities in catalysis**

Learning activities can have vastly different infrastructure requirements, but ST activities do not necessarily demand high-end technologies for their implementation. Consider the use of Think-Pair-Share (TPS), a simple decades-old instructional strategy, in a ST setting applied to the rhodium-catalyzed hydroformylation reaction.\(^{37}\) Figure 5 includes the conventionally drawn catalytic cycle for this process.\(^{38}\) Through TPS, students can be asked to analyze the effect of phosphine ligand concentration, carbon monoxide partial pressure, and olefin concentration, on individual reaction steps, as well as, system-level properties, such as the overall rate of reaction and the ratio of linear to branched alcohol obtained in the product stream (Figure 5). Subsequently, students can be asked to synthesize the set of conditions that would yield a desirable product selectivity at the highest possible reaction rate. The knowledge of how different factors affect the rate determining step in a catalytic cycle is disseminated in current catalysis courses too, but seldom in a manner that fosters ST as proposed in the TPS activity. The learning activity also serves as a platform for students to apply principles of previously learned concepts like chemical equilibrium, thermodynamics and kinetics, to organometallic chemistry in homogeneous catalysis. On a level where we draw the system boundary around the ‘hydroformylation’ reaction, the activity allows for the identification of system components and the interrelationships that exist within. On a larger world systems-level, other considerations need to be factored in; in this case, what is the environmental impact, cost and availability of the different chemicals that feature in this process? And how would these factors reform the catalytic process in the years to come? Such topics are the basis for the third segment of the TPS activity (Figure 5). Therefore, the TPS starts from a reductionist perspective, asking to think about individual reaction steps, and builds towards a holistic perspective, finishing with the consideration of a global system of systems.
Ho pointed to ensemble thinking and ideality as a key challenge for ST in general chemistry education.\textsuperscript{18} The same applies to the field of catalysis too. The derivation of the Langmuir adsorption isotherm and Langmuir-Hinshelwood (LH) rate equations are based on a number of assumptions, which are usually clearly communicated to students. In a next step, they should be encouraged to think of the consequences of relaxing one or more of the underlying assumptions. It is sufficient if students can formulate a qualitative hypothesis for such cases, since the actual derivation of rate equations under these conditions can be more tedious. Nevertheless, even such a qualitative analysis triggers fundamental ST competencies and allows the appreciation of non-ideal behavior. In other words, this activity is aimed at students questioning the assumptions and dissecting their systemic effects instead of merely accepting them as a basis for the derivation of a mathematical expression. Moreover, LH kinetic models should be used more efficiently to demonstrate non-linear effects in catalytic reactions. The rate equations derived under these models can usually be organized into the following general form:

\[
rate \ of \ reaction = \frac{\text{(kinetic term)(driving force)}}{\text{(resistance term)}}
\]

The resistance term in the formula depends on the rate-limiting step, which can be one or a combination of, reactant adsorption, surface reaction and product desorption steps. Even the simplest versions of such kinetic models illustrate the non-linear effects of different parameters on reaction rate. For instance, in the case of hydrogenation of ethylene to ethane over a nickel catalyst, the LH rate equation takes the following form:

Figure 5. Left: Catalytic cycle of the rhodium-catalyzed hydroformylation / oxo-synthesis.\textsuperscript{38} Right: TPS activity to foster ST in hydroformylation catalysis.
\[
\text{rate} = \frac{K_1(K_2 p_{C_2H_4} p_{H_2} - K_3 p_{C_2H_6})}{(1 + K_4 p_{C_2H_4} + K_5 p_{H_2}^{1/2})^3}
\]

Importantly, learners must not be restricted to visualizing non-ideality as emanating from mathematical equations, but instead, must be able to visualize what happens on a systems-level and how that manifests in mathematical formulations. This calls for the diligent preparation of learning activities, where the instructor provides sufficient scaffolding to ensure that students are indeed thinking on a systems-level.

**Themed workshops in catalysis for ST**

Mechanistic-reasoning approach, context-based focus and sustainable-action perspective are listed as the three core elements of chemical systems thinking. Themed workshops as a learning activity can incorporate each of these core elements. Herein, this is illustrated through an example of automotive catalyst systems (Figure 6). The advantages of employing a context-based focus are manifold and themed workshops readily provide a relatable context for students, where they can connect chemistry concepts with issues of global importance. To accomplish the desired ST outcomes, the workshop must enable students to apply catalysis concepts to real-world applications within a framework that helps them connect fundamental and mechanistic reasoning to larger system-level phenomena of vehicular transport and environmental emissions. With respect to the fluid catalytic cracking process in the ‘catalysis in gasoline production’ subsystem, an example of a standard reductionist question is ‘Why is a binder and a filler added to the catalyst composition?’. Now consider the following set of questions: (i) How would the stability of the catalyst be affected if the composition of the binder and filler is changed? (ii) What influence will this have on short-term catalytic performance? (iii) How could changing the binder composition influence catalyst deactivation-regeneration cycles? (iv) Would the product distribution be liable to change on making these changes to the catalyst composition? (v) How is the vehicle engine susceptible to changes in product (fuel) composition? and (vi) Would this modulate the performance of the exhaust catalytic converter and thereby, environmental emissions? These set of questions start from a simplistic cause-effect relationship and sequentially build towards system-level emergent properties closely integrating core heterogenous catalysis concepts along the way. The stream of thinking culminates with an assessment on environmental impact. Moreover, a discussion on catalysis in next generation renewable energy-fueled transport targeting lower carbon emissions is another means to integrate the interaction of catalysis concepts with earth, societal and environmental subsystems. This constitutes the ‘sustainable-action perspective’ component of chemical systems thinking. Particularly, when it comes to discussing catalysis for applications in the future with an environmental perspective, the workshop must bestow students with a degree of liberty to brainstorm ideas and hypotheses. Some of the topics listed in Figure 6
such as fuel cell-powered transport and materials for reversible hydrogen storage are extensively researched worldwide in the present day. Furthermore, the exposure to these topics will shed light on state-of-the-art research methodologies and tools in catalysis research, which would be difficult to communicate if only industrially established processes are chosen for instruction.

Figure 6. A proposal of topics to be explored in a ST workshop on automotive catalyst systems: (i) Catalytic processes for gasoline production in the current oil-based economy (in blue), (ii) Catalyst converters for exhaust emission control (in black), (iii) Catalysts and materials for next generation fuels and cars (in green) and (iv) Assessing the environmental impact of current and future transportation technologies (in purple).

Student assessment of ST competencies in catalysis

Assessment design based on the Systems Thinking Hierarchical Model

For a catalysis course that aims to develop ST competencies, it is insufficient if the assessment only tests the students’ abilities to apply core concepts to reason and explain different phenomena in specific contexts. While there is general consensus that assessments would have to be redesigned to effectively evaluate ST skills, the specifics of how such assessments are to be framed remain topics of discussion in the chemical education research community.

Figure 7. Simplified block diagram of the Total Paraffin Isomerization Process: Linear alkanes are isomerized over a bifunctional platinum-loaded mordenite catalyst followed by the separation of branched alkanes from linear alkanes using zeolite A.

Herein, the Systems Thinking Hierarchical (STH) Model is used as the basis to formulate an assessment task on the ‘Total Isomerization Process’ (Table 1). The paraffin isomerization
process is catalyzed by a platinum-loaded zeolite mordenite catalyst with zeolite A being used as a molecular sieve for the separation of linear from branched isomers (Figure 7). The assessment questions are designed to trigger the eight skills in the STH Model pyramid, which are divided into three levels: analysis of system components, synthesis of system components and implementation.$^{1,5,45}$

Table 1. Sample questions on the Total Isomerization process to test ST skills as ordered in the STH Model.

<table>
<thead>
<tr>
<th>Level of systems thinking</th>
<th>Systems thinking skill</th>
<th>Sample question</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analysis of system</td>
<td>Ability to identify components of and processes within a system</td>
<td>What function does (i) Pt/MOR and (ii) zeolite A play in the sketched process?</td>
</tr>
<tr>
<td>components</td>
<td>Ability to identify relationships among systems’ components</td>
<td>The residence time in the first unit is halved. How does this affect the performance of the second unit?</td>
</tr>
<tr>
<td>Synthesis of system</td>
<td>Ability to identify dynamic relationships within the system</td>
<td>Pt/MOR is found to deactivate after a long time on stream. As a result, how is the operation of the second unit impacted as a function of time?</td>
</tr>
<tr>
<td>components</td>
<td>Ability to organize the systems’ components and processes within a framework of relationships</td>
<td>Comment on the size specificity of the zeolites used in the two units. How does this modulate the overall process performance?</td>
</tr>
<tr>
<td></td>
<td>Ability to understand the cyclic nature of systems</td>
<td>Due to glitches in heat management, the temperature of the first process unit containing Pt/MOR drops significantly. How does this impact the performance of the second process unit and thereby, the recycle load?</td>
</tr>
<tr>
<td>Implementation</td>
<td>Ability to make generalizations</td>
<td>For the loading of Pt on the zeolite, there are two MOR samples available, one with a Si/Al ratio of 8 and another with 50. Which of the samples is likely to provide a superior isomer productivity?</td>
</tr>
<tr>
<td></td>
<td>Understanding the hidden dimensions of the system</td>
<td>The loading of Pt in zeolite MOR of a Si/Al ratio of 18 is increased. How will this affect the performance of the first unit and the process as a whole?</td>
</tr>
<tr>
<td></td>
<td>Thinking temporally: retrospection and prediction</td>
<td>The zeolite in the second process unit is changed to ZSM-5. How does this affect the performance of the first unit?</td>
</tr>
</tbody>
</table>

Table 1 lists exemplar questions corresponding to each level of ST. The most basic ST skill is the ‘ability to identify components of and processes within a system’. With regards to the paraffin isomerization process, the attainment of this primary skill can be checked by asking students to identify the role of Pt/MOR and zeolite A in the two units (components) of the overall process (system). The next set of questions on ‘relationships’ within the system are meant to test ST skills further up the hierarchy. These questions ask students to evaluate the effect of a specific change in one process unit on the other process unit. Also at the level of ‘synthesis of system components’, students can be assessed for their ability to evaluate factors that
influence the recycle stream. Along with testing the students’ ability to understand the cyclic nature of systems, such questions integrate knowledge domains of allied concepts like thermodynamics, which is fundamental to answer questions on how changes in temperature affect the catalyst performance and the process as a whole. At the ‘implementation’ level, questions are formulated to test the ability to make generalizations and predictions; for example, to predict process performance on increasing the Si/Al ratio of zeolite MOR. In the paraffin isomerization process, Pt/MOR is a bifunctional catalyst, where the paraffin dehydrogenation step occurs at the Pt metal site and the conversion of the olefin to a carbonium ion is mediated by a strong Brønsted acid site in the zeolite. When the Pt loading in a zeolite of a fixed Si/Al ratio is increased, it is accompanied by a reduction in the number of Brønsted acid sites. Therefore, increasing the Pt content in the zeolite does not necessarily augment the isomer product yield. The trade-off between the Brønsted acid content and Pt loading in the zeolite constitutes a hidden dimension of the system that students must be able to comprehend (Table 1).

Writing assignment-based assessment of ST in catalysis

Framing writing assignments based on open-ended questions and scenarios can be particularly effective in nurturing ST competencies. Instructors can also be more elaborate in their feedback to students’ essay-type responses. Such writing assignments constitute the best opportunity to employ feedback in a ‘feedforward’ mode, where students submit their first draft, receive timely feedback from the instructor, and then actively revise the first version by deploying the learnings from the instructor’s comments. Consequently, such writing projects may be used both as a form of formative and summative assessment.

Current research topics in catalysis offer good scope for these kind of writing assignments. Not only does engaging students in these topics provide them with their first exposure to research, which is a good thing on its own considering that catalysis course modules are offered to students who are nearing completion of their undergraduate degree programme or at the M.Sc. level, but it also fosters a ST perspective to address research issues. The necessity of holistic thinking is becoming increasing apparent in several hot research topics, such as in the catalytic partial oxidation of methane. A commercially viable direct methane-oxidation technology for operation on a small-to-medium scale remains elusive. A recently published perspective on this topic identifies how every extensively explored approach for methane-oxidation does not simultaneously address core vital issues of product yield, oxidant choice and engineering aspects. The article concludes by saying that “On the whole, a more holistic approach is required to design efficient, novel catalytic processes for this chemistry and to upgrade existing laboratory-scale methods to the industrial scale”. Therefore, it can only be ideal that we encourage the practice of ST in catalysis research starting from the classrooms.
Conclusions and Outlook

As is the case with most general chemistry courses, catalysis course modules are also predominantly taught using a reductionist perspective. While this would come across as an intuitive way of instruction for a discipline that deals with the understanding of phenomena at the molecular level, complementing the traditional ‘zoom in’ approach with a systems thinking ‘zoom out’ approach is paramount to achieve better learning outcomes in students. Previously published studies have highlighted the necessity to engage chemistry students in systems thinking to prevent ‘disciplinary siloing’ of knowledge. The sub-discipline of catalysis is no exception to these observations. However, (re)designing a catalysis course module to achieve systems thinking-based learning outcomes entails different challenges than those for general chemistry courses. The first apprehension that may come to mind when thinking of a shift to a ST approach in catalysis is that the ‘depth’ of chemistry might be compensated in pursuit of the ‘breadth’. However, through multiple examples in this article, we illustrated that the technical rigor of a catalysis course does not need to be diluted when employing a ST focus.

A specific challenge for ST in catalysis education that was discussed in detail in this article was that of rising above contextualized pedagogy. While providing context is undeniably an important ingredient in the recipe of ST, merely introducing and explaining concepts in a contextual background does not necessarily activate ST skills. Herein, through multiple examples, we showed how we can go further to genuinely trigger ST in catalysis.

The scope for implementation of ST in the instruction of homogeneous as well as heterogeneous catalysis is immense: from the creation of ILOs and use of graphical tools to the design of learning activities and assessment tasks. In this article, we touched upon each of these aspects to demonstrate how a rather seismic shift to ST in catalysis education can be achieved. While redesigning a course for the attainment of ST outcomes will certainly require considerable time and effort, not all didactic strategies are tedious to plan and adopt. For instance, the organization of themed workshops of the kind proposed in this article will require elaborate planning but recasting currently delivered content using a ST mould is a strategy that involves minimal effort. It would be worthwhile to start the transition to a ST approach through such smaller incremental steps and eventually progress to the creation of a full-fledged catalysis course grounded in systems thinking. In this context, instructors must strive to transition from the strong petrochemical context of currently taught catalysis content to a more renewable bio-based context. While this article was focused on lending a ST perspective to largely familiar catalytic applications, we strongly advocate extending this approach to biomass valorization catalysis as a next step. As discussed herein, the framework for systems thinking in catalysis will largely still hold, but thinking of world systems-level aspects like circular economy, sustainable feedstock, energy efficiency and environmental impact can be advanced to a higher level.
Since ST is still relatively new to chemistry education, fundamental questions on their implementation continue to exist. Going forward, one such aspect that needs increased attention and clarity is the design of student assessment tasks to assess ST competencies. For instance, to what extent can current summative assessments be modulated to assess ST outcomes? How should grade descriptors be formulated in such standards-based assessments? Furthermore, guidelines for the design of such assessment tasks are yet to be fully established. These are important issues to work on for educators of catalysis and other advanced chemistry courses.

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