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Systems thinking, green chemistry and the molecular basis of sustainability

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Slide	Text
1	Thanks you for the opportunity to speak about some of the work that Peter Mahaffy and I have been doing with others over the last couple of years, about the role of chemistry in sustainability and, in particular, about the importance of systems thinking and how this can be introduced into chemistry through education.
2	From a chemistry perspective, there are three key strands that are involved in the sustainability issue: • Concerns and concepts • Agendas and agreements • Chemistry's roles These three strands have been co-evolving for a long time – not independently, because they are tightly intertwined together and interconnected. And I want to make the point that ***systems thinking*** (ST) is a common thread that makes the interconnections, the cross-links, between these core strands. I don't have time today to discuss this background in any detail, but it is covered in a number of publications that are either already out or about to appear.
3	Regarding chemistry's role: For more than 200 years, discoveries and developments in chemistry have accompanied the developing picture of sustainability, from studies of the physical chemistry of the Earth's atmosphere and the nature of the greenhouse effect in the 18th and 19th centuries to the establishment of Green Chemistry in the late 20th century and the emergence of the new academic discipline of sustainability science at the start of the 21st century. Our group called 'Chemists for Sustainability' at IOCD has promoted an approach we call 'One-World Chemistry', which recognises that the health of human beings, animals and the environment are all intimately connected; seeks to re-position chemistry as a 'sustainability science' for the benefit of society; and embraces systems thinking and cross-disciplinary ways of working. A very important impetus to chemistry's role in sustainability has come from the 3Rs Initiative. Its principles of Reduce, Reuse and Recycle are the core of various established and emerging movements that are trying to reach sustainable development. The familiar 3Rs logo made its first appearance at the first Earth Day event, which was celebrated in the USA on 22 April 1970.
4	Language is itself an important ingredient in determining how and what people think: in an article we put out a couple of weeks ago on Earth Day 2019, our IOCD Chemists for Sustainability group argued that the very concept of waste should disappear from our vocabulary and we should regard all matter as being available for reuse - as 'post-trash' in a sustainable world.
5	It is evident that there are a number of key linkages in all of these concepts and approaches • All recognize interdependence between human activity, human and animal health and the biological and physical environments of the planet. • And it is evident that the potential solutions, such as through prevention, mitigation, clean-up and recycling, will not be achieved without major inputs from chemistry, which can bring understanding of the *molecular basis of sustainability** and to do so it needs to incorporate systems thinking[⊖].

	* The term *molecular basis of sustainability* was used in an article by Paul Anastas and Julie Zimmerman in 2016, in which they spoke about the achievement of green chemistry through design. They emphasised that chemists possess ultimate responsibility for consequences in the design of what they make; and that many of the solutions to the environmental challenges we face are potentially molecular. Θ Systems thinking can be seen as an interconnecting thread that runs through and unites all these approaches to sustainability.
6	We consider this term, *the molecular basis of sustainability*, especially relevant to describing the role and ambition of chemistry and have therefore adopted it and extended its application, more broadly, to include *"the ways in which the material basis of society and the economy underlie considerations of how present and future generations can live within the limits of the natural world.*" The term recognises that science of chemistry is concerned with analysing, synthesising and transforming matter, i.e. the material basis of our world; and it clearly establishes need for both the practice of chemistry and education in and about chemistry to address sustainability of earth and societal systems.
7	In 2017 we initiated a project with the International Union of Pure and applied Chemistry, which is also supported by IOCD. This project involves a global team of about 2 dozen leading chemistry educators. It aims to infuse systems thinking into mainstream chemistry education. The intention is to help chemistry students to acquire a more holistic view, equipping them to be better able to: ➢ understand chemistry: ➢ engage in cross-disciplinary work: and ➢ address emerging global challenges: In the course of this project, in which we have held dialogues with chemistry educators from around the world, some of the key feedback we have received has concerned the need to develop materials and examples to support the teaching of systems thinking in chemistry. One of the most important aspects of this has been the demand for visual materials to help guide the process of systems thinking. In the rest of this talk, I want to give you a brief summary of how that has been developing, using examples drawn from the Planetary Boundaries approach.
8	So, let's begin with an example based on the Planetary Boundaries concept and take look at climate change.
9	By 2015, the value of the CO_2 indicator for this Planetary Boundary variable was already above the threshold level of 350 ppm and currently stands at around 412 ppm. How can the biogeochemical flow system that this number represents be made clear and relevant to the chemistry learner?
10	One visualization technique that has been extensively used to explore systems effects is the Concept Map. This tool was pioneered by John Novak in the 1970s and 1980s. As illustrated in this example, the Concept Map uses boxes with Concept Labels, which can be objects, ideas or effects, and arrows with descriptions to depict the relationships among the Concept Labels. There is generally a flow of effects as one progresses down the map.
11	So, if we apply this approach to look at the biogeochemical flow of CO_2, we might begin the Concept Map something like this… … and see how the chemical and biochemical process that generate CO_2 lead to an elevated concentration in the atmosphere and explore the chemical changes and the physical and biological impacts on land, sea and air. But we felt a need to make the visualisation even more system-related and be able to define domains of particular focus for chemistry, so we have developed a systems-oriented extension of the concept mapping tool in order to do this. Rather than continue with the CO_2 issue, I will illustrate this with a different example related to another biogeochemical flow.
12	What is the most important technological invention of the 20th Century? Many people may be tempted to say the computer microchip or the internet. But a strong case can be made for the chemical reaction that took place in this apparatus over 100 years ago, and which has been scaled up to this manufacturing plant. This reaction is the **Haber-Bosch Process** for the synthesis of ammonia. A modern plant will typically produce 1,000 to 3,000 tonnes per day of ammonia. About 85% of total world production is used in agriculture. And this is the reason that this chemical is so important. As Vaclav Smil has pointed out, around 40% of the current world population depends for its existence on agricultural products that have been enabled by the use of N fertilizers and the number is bound to increase as the planet's population keeps expanding.

13	But unfortunately, this is not a simple story of success. The Haber-Bosch process has helped feed the world for the last century – but it can also be seen as a failure of systems thinking in chemistry. And there are at least three reasons for this: 1. Making and using N fertilizer has a high energy demand. So, in 2017, the production of this single chemical, ammonia, accounted for 1.8% of global fossil fuel consumption. 2. The use of ammonia-based fertilizer is extremely wasteful of N. So, in the production of crops for a vegetarian diet, for every 100 atoms of N in the fertilizer produced, only 94 are actually applied on the field; only 47 find their way into the crop, and after, harvesting and food preparation only 14 N atoms are actually consumed. The situation is even worse for a carnivorous diet, where out of every 100 atoms of N in the fertilizer produced, only 4 N atoms are actually consumed in the meat that is eaten. 3. Making and using N fertilizer also causes widespread damage to the environment, including air, land, sea. To see how this happens and relate it all to chemistry and to chemistry education, we can again begin with the planetary boundaries…
14	and we see that the biogeochemical flow for N is already well into the red zone…
15	The Planetary Boundary for N was set at 62 Teragrams per year, and the value of this indicator was estimated in 2015 to be already about 2½ times that amount. So we are already greatly exceeding what is considered to be the carrying capacity of the planet for reactive nitrogen, and the demand for food can only be expected to grow steeply in this century as we add another few billion people to the world's population.
16	So let's now look at some of the ways that chemistry is situated in this picture. And I will now introduce our new visualization tool, the systems-oriented concept map extension or SOCME, to illustrate the process. We start with the core reaction system of the Haber-Bosch synthesis. Chemistry teaching usually focuses on the stoichiometry of the reaction between hydrogen and nitrogen to give ammonia; and on the reaction control conditions, which we can explore by developing a Reaction Conditions Subsystem.
17	The reaction requires a catalyst, which in the industrial synthesis is iron-based, and requires high temperature and pressure to drive the equilibrium towards product formation. Chemistry teaching usually focuses strongly on this equilibrium element, using the opportunity to introduce and explore Le Chatelier's Principle.
18	So, what if we begin to take this further, and consider the Energy Input Subsystem? As I mentioned, the industrial Haber-Bosch process is responsible for nearly 2% of the world's hydrocarbon fuel consumption. Typically, more than 60% of the total production cost of ammonia is accounted for by the hydrocarbon feedstock. One use of this fuel is to provide the energy that drives the compressors and heaters needed for the reaction conditions…
19	But we also should look at the Chemical Input Subsystem and ask where the reactants come from. In the industrial Haber-Bosch process: • the source of nitrogen is from the liquefaction of air • the source of hydrogen is from the cracking of methane and other hydrocarbons to produce 'synthesis gas', in a sequence of reactions with water that also require high temperature and pressure. • You will note that CO_2 is one of the other products of this process – and of course, it is also produced by the combustion of the hydrocarbon fuels to provide the energy for the core reaction to synthesise ammonia. Up to 3.5 tonnes of CO_2 is emitted for every 1 tonne of NH_3 produced. The CO_2 is traditionally expelled into the atmosphere, and this therefore connects to the biogeochemical flow stream for CO_2 and climate change. Rather than explore the CO_2 SOCME today, I will stay on the fertilizer track and take us in the direction of the Ostwald Process Subsystem.
20	The Ostwald process is used for making nitric acid by the sequential oxidation of ammonia. Here the chemistry class can explore the oxidation states of nitrogen and the chemical properties of nitric acid, including the formation of the soluble nitrates. It can also explore acid-base chemistry in the reaction of nitric acid with ammonia, to form ammonium nitrate, one of the most widely used N fertilizers.
21	So, we can progress into the Intended Uses Subsystem, which has two very major components: the applications in agriculture and explosives • Over 80% of the ammonia produced globally is used in agriculture. N fertilizers are a major source of the organic nitrogen compounds which are essential for life. But as we saw earlier a high proportion of the N in the fertilizer is lost along the way and much of it ends up on the land and in the water and also, through oxidative processes, in the atmosphere, where nitrogen oxides act as indirect greenhouse gases.

	• The second largest use of ammonium nitrate is in the manufacture of explosives, which are used in munitions, mining, colliery and civil engineering. In this sub-system the chemistry class can explore the biogeochemical pathways by which nitrogen compounds are oxidised, reduced and metabolised, as well as the high-energy properties of some compounds and the chemistry of explosives….
22	… and it can also give attention to the unintended consequences that arise from these uses, in which environmental nitrates contaminate land and water supplies; and in which explosives are used in conflicts.
23	Valuable attributes of the SOCME include that • it encourages expanded thinking about which subsystems to explore for a specifically tailored chemistry course, and thinking about what happens if the boundaries are expanded to include other considerations; • it also facilitates thinking about what happens if a particular subsystem or group of subsystems is replaced by an alternative. So, for example, we might consider what would be the consequences if we did not use hydrocarbons as the source of the energy and the hydrogen for the Haber reaction…
24	One of the alternatives that has been used to support the Haber-Born process has been hydroelectric power for the electrolysis of water to produce the hydrogen, in countries where surplus hydroelectric power is available – like Norway and Iceland. Current work is also going on to develop photochemical methods – capturing the energy from sunlight to split water. And there is also research being undertaken to find catalysts that will enable the splitting of water to produce hydrogen under mild conditions; and to catalyse the reaction between hydrogen and nitrogen to take place under much milder conditions of temperature and pressure than in the classical iron-catalysed Haber reaction. Each or these options will require consideration of the reaction control conditions.
25	Of course, none of these options will affect the results of using ammonia through the ammonium nitrate pathway. But we can consider that separately through another set of subsystems. For example, we can examine what happens when the urea pathway is used instead. Urea has the advantage of being a more intense carrier of nitrogen and can be employed both as a fertilizer and as a source of urea-based explosives. More than 90% of world industrial production of urea is destined for use as a nitrogen-release fertilizer. Other applications include urea-based explosives and urea-formaldehyde resins used in plywood manufacture. These applications will again have both intended and unintended consequences that need to be explored.
26	Last year, the Journal of Chemical Education accepted our proposal to have a Special Themed Issue on Systems Thinking and Green and Sustainable Chemistry and a call for papers was published. Several dozen papers have been received and the Special Issue will be appearing around the end of this year.
	Finally, on behalf of Peter and myself, I would like to acknowledge the contributions by our funders – IUPAC and IOCD – and by our colleagues in the STICE project group, and encourage you all to look out for the forthcoming Special Issue of the Journal of Chemical Education.