Next Generation Research Podcast

Episode 3: Catalysis makes the world go round: understanding how our society depends on industrial chemistry

Giles: Does the climate crisis and our use of fossil fuels worry you while you are driving? Does it feel overwhelming? thought about electric cars? Me too. We need to make big lasting changes as a species in order to curb the effects of climate change. Net zero is a term you may have heard in the news before, but what does it actually mean?

Giles: The term was coined by the United Nations, but it means different things in different countries. In the United Kingdom, the goal by 2050 is for the amount of greenhouse gas emissions produced to be equal or less than the emissions removed from the environment by the uk.

Andrew: What's the most motivating part of chemistry to you as an individual? And that's really about solving problems associated with. Sustaining the quality of life that we have whilst also minimizing the impact on the environment around us. And that's where things like Catalysis are vital.

Giles: This episode is about how a process called Catalysis could be a key part in making net zero a reality. Welcome to Next Generation Research, where we bring you the most important and exciting research happening at the moment. I'm Professor Giles Yeo, a scientist from the University of Cambridge, and in each episode I have the pleasure of introducing you to one of the best researchers working in the UK right now.

Giles: All of them are part of the Future Leaders Fellowship. They are all working to solve problems and improve our lives as we know them. This episode is about the research and collaboration being done to improve the way we make lots of necessary products for human life. The voice you just

heard is Dr.Andrew Logsdail, a senior lecturer in catalytic and computational chemistry based at the Catalysis Institute at Cardiff University. [00:02:00] Before we go any further, let's remind ourselves what a catalyst is. A catalyst is something which increases the rate of a reaction, but is not used up in the process itself.

Giles: It often means the reaction can take place with lower energy requirements. For example, you may have heard about the catalytic converter in your petrol car. It sits near the engine and is coated in precious metals such as platinum and palladium. When it heats up, the toxic chemicals produced from your engine, such as carbon monoxide, pass over these precious metals and are converted into carbon dioxide and water.

Giles: This is a good thing as we don't want these toxic chemicals in our atmosphere, but as I'm sure you are well aware, we also have far too much carbon dioxide in our atmosphere, and Andrew and his colleagues are trying to do something about that. His research fellowship is all about coming up with new ways to use computer models to work out how catalysts can help us make portable fuels, which are better for the environment.

Giles: These are the sort of fuels we use in cars, lorries, and ships. Andrew's work is a combination of computer science, physics, material science, and chemistry. He designs computer models to test potential catalysts, and he can give that information to his colleagues to take into the lab for experimentation.

Giles: As you'll hear, collaboration across disciplines is crucial when it comes to solving problems such as how do we reduce the emissions from transport and industry, and how do we do it quickly?

Andrew: So what we want to use or what we wanna find is this material which we can use to accelerate a reaction, which doesn't get used up itself

in the reaction so that we can just use it over and over again without impact on the productivity of our process.

Andrew: It's what Catalysis provides us with is a way to make consumer goods in a less environmentally impactful way. Catalysis has lots of applications in our society. One of those is fuel. Another one, which is huge, would be the design of catalysts for making ammonia. So ammonia is vital to the sustenance of half the population on the globe as a fertilizer or as a feeder fertilizer synthesis, we want ways to make ammonia as efficiently as possible.

Andrew: Currently, ammonia consumes a significant amount of the global energy supply and of our fossil fuels because of the fact that we use hydrogen generated from fossil fuels to make ammonia. We use catalysts to make them at the moment, but we need new catalysts. And we need new catalysts, which allow us to use hydrogen from renewable sources and activate nitrogen, which is the two key elements inside of ammonia, to then give us this really valuable fertiliser that the world depends on.

Andrew: And what I've done is look about how we can solve these chemical problems as quickly as possible and give us as much information with computing. Computational research, which we do, is really focused on basically supporting experimental work by using computers. We use foundational equations from physics and we put them into software that has been implemented in computers, and we're thinking about how we can efficiently solve these equations on these really big computers to tell us about the applied chemistry.

How can we predict how molecules interact with each other? How can we predict how they interact with catalysts? And then how can we understand which of the best catalysts we wanna use catalysts to provide ourselves with energy, which we can use to drive around our cars.

Andrew: we all know that we don't want to use combustion engines forever because they have an environmental impact, but we do know that. At the moment, we need to continue to use those till we find something suitable to replace them. So synthetic fuels are gonna be a very important part of our near future.

Andrew: What we are thinking about is how we can create those synthetic fuels. Can we take things which are seen as environmental pollutants? So carbon dioxide for instance, which has a carbon molecule, which is important in terms of fuels, and can we turn that into a fuel which we can put into your car. Carbon dioxide is a really challenging molecule to turn into anything useful because it's really stable.

Andrew: That's why it's such a big environmental problem. What we're working on is finding these catalysts, these materials that interact with carbon dioxide. And actually what we found is just getting carbon dioxide to interact. A tool is a real challenge. That means we've gotta go through all these different combinations of catalysts, these materials which could interact with carbon dioxide.

Andrew: And we found that if we change round the different compositions of our materials, so we change elements in and out, we can find somewhere carbon dioxide does interact with the surface. And when we get an interaction, then we can start to change it into different molecules. With the outcome at the end of it being this, this methanol, this, this target molecule we're interested in.

Giles: Andrew and his colleagues know they're looking for something which helps turn carbon dioxide into methanol, but there are so many possible materials that might make this work, and this is where Andrew's computer models come in to help speed up the process.

Andrew: We run all of this through the models. We can test hundreds of different compositions.Hundreds of different material structures as well. What we'll see is the differences in processes with different catalysts, and we'll look at those and we'll see, well, which one's gonna give us what we call the lowest barrier to perform that reaction. And with that, we can then say, that's gonna be the best, that's the most efficient process.

Andrew: Let's give that to our colleagues in experimental labs. And what you've got is an efficient way of screening, so they don't have to do all of the complicated testing for all the different elements. They can just take the best predictions, use those. And then run the experiments and come back and tell us that we've got it wrong.

Andrew: One of the researchers who's doing really great work on this is Naomi Lawes, who's based here in the Cardiff Catalysis Institute working on the experimental side of this project.

Naomi: Catalysts are key in industry. Over 90% of industry uses them. They are essential for our society to function. We wanna tackle climate change.

Naomi: We know that carbon dioxide is a greenhouse gas, and the aim is to remove this from the atmosphere or this excess CO2 that we have that is damaging our environment and we wanna convert it into something useful like a liquid fuel. And in the process of doing this, we can reduce the dependency on fossil fuels.

Giles: Naomi Lawes is a final year PhD student at the Cardiff Catalysis Institute. She investigates catalysts for the conversion of CO2 into methanol, so it can be used as a fuel.

Naomi: The pros of methanol is that it doesn't produce all these pollutants like petrol, so we don't produce nitrous oxides, sulfur oxides, and essentially it's a cleaner way to burn fuel and we can recycle it back. So where my

research fits in is once the CO2 is captured, we need a catalyst to convert that CO2 into methanol. If we didn't have a catalyst, we wouldn't be able to run the reaction. We need to use the catalyst to help make this process more efficient, to make it feasible at lower temperatures, at lower pressures.

Naomi: And also it helps with the selectivity. If we convert co2, you can get various products that we might not necessarily want. So to make a reaction more efficient, you wanna select the desired product, the one that you're after. So I make a catalyst, which essentially is a gray powder, and I make this in labs, and we can use a reactor to input the carbon dioxide, and this will run over our catalyst, which can convert that into methanol.

Giles: The collaboration with Andrew's team is vital and also symbiotic with Naomi's work.

Naomi: I've worked with the computational team here at the Cardiff Catalysis Institute to optimize what catalyst I could use. So if we didn't have the aid of computational chemistry, it would feel much more of a trial and error task.

Naomi: Computational chemistry can really narrow down the available material and suggest what material is most stable, which is favorable, and then we can synthesize that in the lab and test it. We can feed in material that we think could work. And from testing in labs, we might see an outcome that hasn't been predicted yet, and we can feed that back to the computational chemists and they can add that into their modeling.

Naomi: And that can help feed us further in labs. So it's definitely about the two-way relationship between computational and experimental chemistry.

Giles: When people like Naomi have finished doing their experiments, Andrew's team can take that feedback and understand even more about what they've predicted.

Andrew: We essentially start with a hypothesis where we're testing that hypothesis to give the prediction.

Andrew: And it could be that we run the experiments and our hypothesis is wrong. So that could be, for instance, that carbon dioxide interacts with the surface in a different way that we thought it would. We just said, all right, it just lies down on top of it. But actually it doesn't do that. So then what that means is we go back to our computer and we go, okay, let's look at the different orientations that we can have for this molecule on this surface, and the different ways that we could say, for instance, add hydrogen atoms onto it to form the fuel we want.

Andrew: And we take that and we then run those tests again and then go back to the experimental team and say, well look, does this fit your data better? If not, can you run experiments further to try and understand it? For us, we can tighten the funnel that we're searching within. And we can do that same process again and again until we get to a point where we have a convergence of the understanding for the chemistry we're interested in.

Giles: This is science, after all. We almost never get something to work the first time. It is always an iterative process.

Andrew: If we iterate and we get convergence and they say, well, the mechanism that you've proposed is the one that we can see from our experiments. That's elating. That's a really satisfying feeling because it means that we can not only create new models, but we can also apply those models and find out new chemical understanding, which then takes us forward in this process of, of development.

Andrew: One really good example of where we've come to this convergence is for catalysts, for making hydrogen peroxide. It's about the synthesis of bleach. So how can we make bleach on location to use it immediately rather than porting around in big trucks, for instance. So in collaboration with Dr. Jennifer Edwards here at the Cardiff Catalysis Institute, we've been able to combine, experiment and computation to find out how these catalysts work and what is the best composition for their application.

Jenny: I think where my research is really focused on the moment is the potential that Catalysis can have in global health applications. So we are interested in how we can use technology that's traditionally been used to sort of benefit the chemical industry to provide more immediate solutions for global health.

Jenny: So I'm Dr. Jenny Edwards, and I'm a senior lecturer in physical chemistry at Cardiff University, but also part of the Cardiff Catalysis Institute. I essentially design and synthesize supportive metal catalyst processes that already would occur. We can use a catalyst to make that process occur at much lower temperatures or lower pressures, and this can be used for a range of sort of industrial reactions.

Jenny: So something that I've worked on has. Been hydrogen peroxide synthesis, which is taking hydrogen and oxygen to gases together and using our catalysts to make hydrogen peroxide. We can look to literature, but if you're thinking about developing new catalysts and innovative formulations, you really need to understand the interactions between metals and the interactions they have on the chemicals that you are looking to transform.

Jenny: The combinations become huge when you consider how big the periodic table is, so that's where theory becomes very important. It saves us time.

Giles: There is a limit to the number of catalysts that you can ever make because funding is limited.

Jenny: So synthesising a single catalyst can take up to about two days, depending on which preparation method you use, and that's to make a single catalyst.

Jenny: So where computational chemistry can really help us is given us an idea of the metals that we should be looking at and the synthesis strategies that we should be looking at, and they can get that information a lot more quickly than we can if it takes two days to make a single catalyst. And we don't even know until we do extensive characterization that we've actually made what we're looking to make.

Jenny: So this idea of how Catalysis can help with disinfection is something that we've been looking at for quite a while. One of the problems with commercial hydrogen peroxide manufacture is this reliance on the infrastructure. So it's made centrally at megaton plants, it's concentrated up, which has an energy cost.

Jenny: It's then shipped to wherever it's being used, where it's diluted back down again to one or 2% at the point of use. Our method of manufacturing would allow it to be synthesised wherever it's required, as long as you have oxygen and hydrogen, which you can get from water and a catalyst. So we've done some work looking at the disinfection properties of our system, of our hydrogen peroxide system, and we find that we get very good disinfection properties if we pass dirty water through the catalyst.

Jenny: At the same time as we're making peroxide, it gets rid of the bacteria very, very well. We have a new project that started about 18 months ago where we're looking at how we can use a photocatalyst. A photocatalyst is a material powder in our case that when it becomes irradiated with sunlight, you get an excitation within that powder, so you end up with a positively charged area and a negatively charged area.

Jenny: Those charged areas can react with oxygen or water to form free radicals. Free radicals are very potent disinfectants and potent molecules that are capable of doing quite difficult chemistry. So things like if you've got chemical contamination in water, you can use free radicals to reduce that down to less harmful products.

Jenny: CO2 and water. That's what we use our photocatalyst for, and in this application we are interested in how we can stick the photocatalyst into a textile. So you have a reusable textile that doesn't really look like it's changed compared to the untreated textiles. And the application we have for that is in reusable sanitary items, menstrual products in areas where people have very limited access to clean water.

Jenny: So essentially you've got a material that you put it out in the sun and it. Disinfects it deodorises and it detains without the need of any water. So it's essentially washing without a washing machine, if you were to clean without washing machines. We're also investigating how we can use this technology and in water cleaning for areas where there's been sort of a tsunami in access to clean water is really limited, is how we can use these types of transformations and these types of catalysts to help immediately in those types of situations.

Giles: Some of those examples actually sound like science fiction. It is so exciting to see how close to reality some of these actually are. As this type

of collaborative research grows. Andrew is also keen to make sure that they are keeping their environmental impact as low as possible.

Andrew: Historically, atomistic modelling on supercomputers in the UK consumed roughly half of the capacity, so that meant half of the biggest computers were used just for modelling of atoms and electrons in the way that we are thinking about in this work.

Andrew: Whilst that's really exciting in terms of what we can achieve, there's also got a big energy footprint. We all know that it takes electricity to run a computer in your house, multiply that out, and you've got a big bill. And so you've gotta think quite carefully about the justification for why you're running these calculations.

Andrew: Now that justification can be made in terms of things like the benefits, when we get this convergence at the end of our results, the prevention of any accidents, because of the fact that we can do it in a much safer environment. If we do something on a computer, we don't have to do it in the lab, so we don't expose anyone to any dangerous situations.

Andrew: There's a lot of work going on in terms of improving the way that we compute things. And so actually at the moment, the next generation computers are gonna have lower energy consumption, and that means actually we have to now adapt. Our programs are our calculators, if you like. And so there's a lot of effort in the field to make computer programs more efficient, to adapt to these new computers, which will come online too.

Giles: Alongside the improved efficiency in computing, Andrew thinks other technical developments will also help bolster this type of research.

Andrew: I am really excited about what we can start to achieve now, really with the improvements in computing powers. When I started working this

field, what, so 20 years ago now, which makes me feel very old, I worked on the presumption and one of the motivating things for me was that I always thought computers are never gonna disappear.

Andrew: The use of a computer has just grown at an astonishing rate, and it's really empowered us in terms of the research we can make, the more efficient computers, and then the introduction of artificial intelligence. The two things which are really pivotal in, in kinda the future of our work with bigger computers or more efficient computers, as has become the case, we can perform larger calculations.

Andrew: Now, larger could mean we can do more calculations of different materials, different catalysts. Larger can mean that we can do bigger models, we can put more atoms in there, or larger can mean that we do them over timeframes. And actually one of the most exciting ones that we're really keen on is the dynamic behaviour of molecules in atoms.

Andrew: So we often think in a chemistry space that when we put something on a surface, it's just a static model. It's like looking at a painting on the wall that it's fixed in the concept that we have. But the reality is that everything is moving all the time and everything is evolving all the time.

Giles: So what are some of the things we can do in our future with this improved technology or with the help of ai?

Andrew: We can study the behaviour of a material, of a catalytic reaction of a catalyst and catalysis over a period of time.

Andrew: We can do that as a function of say, temperature, of pressure, and we can consider how things change. That then gives us this much closer alignment with how. The reactions are going on in the experiments, what we would call a kind of in situ measurement that is then really supported

by artificial intelligence because artificial intelligence similarly gives us this opportunity to just accelerate things.

Andrew: Artificial intelligence will play a pivotal role in our future because we are only creating more data, and as we store that data, when we use that data, we're gonna give ourselves the opportunity to accelerate the ideas. And the knowledge that we can investigate. So all of a sudden we don't have to do a big calculation to figure out some property of some system.

Andrew: We can do a very quick calculation with artificial intelligence. So now we can do a hundred quick calculations for the cost of one slow calculation. So the opportunity here to study these kind of complex, dynamic materials, dynamic reactions, is the new landscape that we're, we're pushing towards. I do this research because I think I hope that I can make an impact on society.

Andrew: I certainly started on it because I thought that that impact would be a direct scientific impact, but nowadays I tend to also think of it as being one where I can impact others and their development and their impact and contribution to solving this problem as well. Research for me is now more about research leadership, where it's about supporting a team and their development, not just answering a question on its own.

Giles: It is clear we need to reduce the CO2 that we're emitting. And yes, we could stop industry. Yes, we could stop driving, but I guess pragmatically, how do we try and save the planet without crashing the economy and putting everyone out of a job? And I think that's an important question to ask. How do we get from where we are now to net zero to having no emissions at all. And this is where the work that Andrew is doing comes in. How do we put together models? How do we put together new technologies? And I think it is important that we be pragmatic in the way

that we are designing solutions for the new world. The other exciting thing as these technologies that are being developed to take us from CO2 World to net zero can be used for so many other things for the benefit of humankind.

Giles: Thanks so much to Andrew, Naomi, and Jenny for taking us around their research world. If you wanna find out more about the Cardiff Catalysis Institute, we've included their website on the episode notes.

And join us next time when we visit Zimbabwe to find out what's stopping people from taking medication to prevent them from contracting HIV.

Valentina: At the moment, there are 38 million people living with H I V in the world, and over half of them are in Eastern and southern Africa. In Zimbabwe specifically, one in eight people are living with H I V and the number of new cases is substantially higher among young girls, and so that's why we really think it's important to focus on them.

Giles: This podcast is supported by the Future Leaders Fellows Development Network. You can find out more about the Future Leaders Fellowship by following @FLFDevNetwork on Twitter, and we will link to their website and our episode description. I'm Giles Yeo, and you can follow me on Twitter and Instagram @GilesYeo.

Giles: The producer is Hester Cant, the executive producer is Freya Hellier. The sound engineer is Morgan Roberts. And thanks to Oliver Mytton and Laura Carter for their additional support. Thank you for listening to this episode of Next Generation Research. Please share this episode with someone who might find it interesting and we'd love for you to give us a rating or review wherever you're listening to this.