



# Clay Materials Show Promise as Fuel Gas Purifiers

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Dr Matthew Lasich

# CLAY MATERIALS SHOW PROMISE AS FUEL GAS PURIFIERS

Finding new and improved methods for purifying fuel gases, to both improve their efficiency and reduce their environmental impact, is an active area of research. **Dr Matthew Lasich** at Mangosuthu University of Technology in South Africa has been utilising computational modelling to discover how clay-based materials can increase the efficiency of fuel gas derived from wood and also reduce the amount of hydrogen sulphide found in natural and landfill gas.

## Purifying Fuel Gas

Natural gas and gas collected from landfills contain complex mixtures of combustible and non-combustible substances. Both are mostly made up of methane and other hydrocarbons with carbon dioxide and hydrogen sulphide being the other notable components.

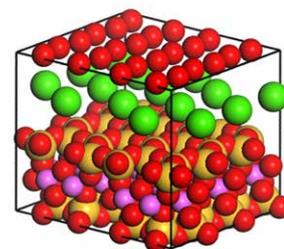
Access to natural and landfill gas is limited for many rural communities. Synthetic gas, or more concisely 'syngas', is one of a few potential substitutes. Syngas can be produced locally from the partial combustion of organic matter with limited amounts of oxygen to produce a mixture composed primarily of carbon monoxide and hydrogen.

While the use of natural, landfill and synthetic gas is widespread, there remains room for improvement. The composition of syngas, for example, is rarely tuned to optimise its energy availability. Natural and landfill gases contain harmful levels of hydrogen sulphide, which has damaging impacts on both human health and the environment. In the presence of

water, hydrogen sulphide can also crack processing plant pipes, increasing maintenance costs.

Dr Matthew Lasich of Mangosuthu University of Technology in South Africa applies computational techniques to design more sophisticated gas purification methods. The work described here focuses on Dr Lasich's computational simulations, which show how synthetic gases can be purified to optimise their energy output, in addition to how natural gas can be purified by removing hydrogen sulphide.

Such computational simulations provide highly targeted sets of results at much reduced costs compared with experimental results. Perhaps more importantly, such modelling techniques can be applied to chemical systems that are unsafe or simply inaccessible. 'We apply computer simulations to study systems in a more controlled manner than is possible in the laboratory,' explains Dr Lasich. 'In this way, we can gain insights that might be difficult to observe.'



Key to the success of Dr Lasich's purification methods is a clay known as 'bentonite'. Bentonite is readily available in many regions of South Africa and can effectively separate gaseous substances. The mechanism of action between bentonite and a gas is very similar to the process that occurs in the catalytic converter of commercial vehicles. As the gas passes over the surface of the material, some of the gas molecules stick to the surface, in a process known as 'adsorption', forming a relatively strong bond. In this example, bentonite is the solid material, and performs the role of an 'adsorbent'. The degree to which gases adsorb onto bentonite depends on the surrounding temperature and pressure, the nature of the gas and the chemical properties at the surface of bentonite.



### **Improving the Energy Output of Syngas**

Wood gas is a form of syngas derived from timber, and is mostly made up of hydrogen and carbon monoxide. This renewable fuel can be prepared using small generators, which can provide energy to local communities that have limited access to other, more conventional forms of energy.

Dr Lasich's recent computational study simulates how wood gas can be refined to increase its energy output per kilogram of gas, by passing the crude gas over bentonite. The clay material can remove the non-combustible components of wood gas, such as carbon dioxide, resulting in higher proportions of combustible carbon monoxide, hydrogen and methane.

Dr Lasich applied a procedure known as 'pressure swing adsorption', where gases passed over an adsorbent are separated under pressure according to how well they can attach onto the surface. Dr Lasich simulated the adsorbent characteristics of bentonite at a temperature of 700°C and pressures

of up to about 10 times atmospheric pressure. While these conditions would be considered modest by industrial standards, Dr Lasich wanted to establish methods that would be more suitable for domestic users who are unlikely to have access to industrial grade systems.

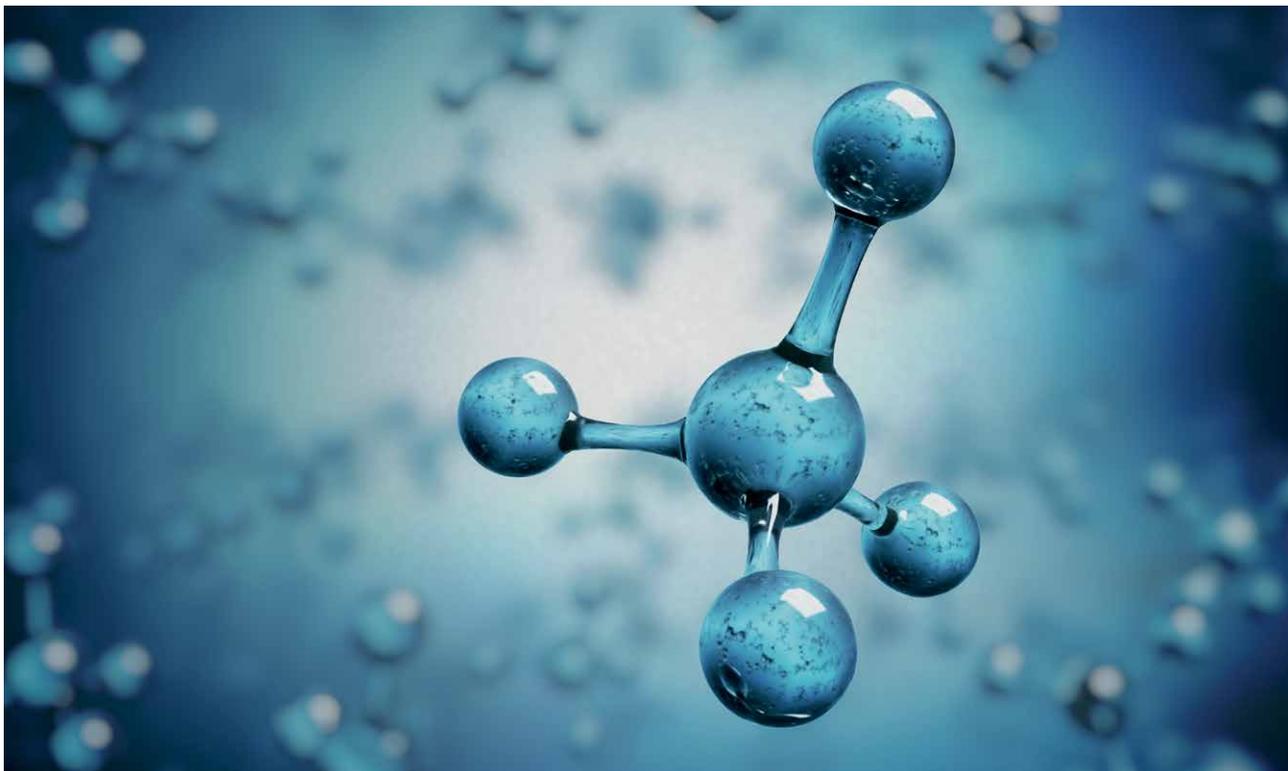
After performing multiple simulations, Dr Lasich found that as pressure increased, the extent to which each gaseous substance adsorbed to bentonite also increased, with hydrogen and oxygen adsorbing more readily than carbon monoxide and methane. This shows that the refined wood gas would contain higher proportions of methane and carbon monoxide, and lower proportions of hydrogen and oxygen. A statistical analysis of the results showed that the energy output per kilogram of wood gas increased by five percent. Over widespread use, a five percent improvement would be very significant.

'Our most important achievement has been demonstrating that a relatively common material – bentonite clay – can provide a boost to the energy content of renewable wood gas using a low energy process,' summarises Dr Lasich.

There are a couple of caveats to note. Dr Lasich explains that the pressure swing adsorption procedures needed to increase the energy content of wood gas may be compromised to some extent by the loss of gas during purification. In this case, he notes that a wood gas recycling system may be required. Furthermore, removing all the oxygen is not always desirable, since an oxygen supply is needed in the combustion of methane and carbon monoxide. In other words, more of the refined wood gas could pass through a combustion engine and be wasted because there was less oxygen available prior to combustion.

### **Removing Hydrogen Sulphide**

Natural gas contains appreciable amounts of hydrogen sulphide, which is poisonous to human health and the natural environment. Therefore, finding new and efficient methods of removing hydrogen sulphide from natural gas is worthwhile. Other research teams have previously published work demonstrating the potential use of bentonite as an adsorbent of sulphur-containing compounds. Following similar lines of inquiry, Dr



Lasich conducted a computational study to find out how well bentonite can adsorb hydrogen sulphide from a natural gas-like mixture. In particular, he explored different bentonite-based materials to find one with a high affinity for hydrogen sulphide and a low affinity for other molecules found in natural gas.

One way in which researchers can modify materials is through a process known as 'doping'. With doping, materials are coated or impregnated with small quantities of a certain element – referred to as the 'dopant'. The inclusion of dopants in bentonite changes how the surface of the adsorbent responds to nearby gas molecules and subsequently, how readily gases are adsorbed.

Dr Lasich conducted a study to investigate the utility of bentonite doped with metal ions, applying conditions that mimic the typical composition of natural gas: carbon dioxide, methane, nitrogen, ethane and hydrogen sulphide. Dr Lasich performed simulations to find out how well the gas molecules adsorb to bentonite doped with either lithium, sodium or potassium atoms.

According to Dr Lasich's results, only methane, hydrogen sulphide and nitrogen adsorbed to the doped bentonite. Furthermore, he found that hydrogen sulphide adsorbs very strongly compared to methane or nitrogen. This result is encouraging because it shows that bentonite is far more selective to hydrogen sulphide compared to all other molecules present in a typical natural gas mixture.

Upon further investigating the results, Dr Lasich found that the extent of adsorption depends on the physical size of the dopant

atoms and the nature of the forces of attraction between the adsorbed gas molecules and the surface of the doped bentonite. His research shows that potassium, the largest of the three elements used as dopants, yielded the strongest interaction, and that hydrogen sulphide, the heaviest gas adsorbed, also formed the strongest interactions. These data all support the idea that large molecules and atoms tend to form the strongest interactions.

Considering the overall results of the study, the dopant that possesses the greatest ability for removing hydrogen sulphide is potassium, followed by lithium and then sodium.

#### **Future Technologies**

Dr Lasich plans to further his research on many fronts. For example, he hopes to improve 'carbon capture' methods, where carbon dioxide is removed from flue gas before it is released into the atmosphere. As carbon dioxide is the primary driver of global climate change, this technology would have profound implications for climate change mitigation. There are also many other minerals to explore, some of which could perform equally well or better when compared to bentonite.

As the global demand for energy increases, more efforts will be required to identify efficient sources of energy that can be used by disadvantaged rural communities, with reduced impact on the environment. In this search for clean and equitable energy, the research contributions of Dr Lasich will no doubt prove invaluable.



# Meet the researcher

**Dr Matthew Lasich**

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Dr Matthew Lasich received his PhD in Chemical Engineering in 2015 at the University of KwaZulu-Natal in South Africa, after which he continued his research with a two-year postdoctoral position. During his PhD studies, Dr Lasich also worked as a visiting researcher at the University of Paderborn in Germany. In 2017, he moved to Mangosuthu University of Technology in South Africa to take up his new role as a Lecturer of Chemical Engineering, and co-founding the Thermodynamics, Materials and Separations Research Group before being promoted to Senior Lecturer in 2020. Dr Lasich is an Affiliate Member of the South African Institution of Chemical Engineers, a Member of the Golden Key Honours Society and an Affiliate Member of the Institution of Chemical Engineers.

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## FUNDING

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## FURTHER READING

M Lasich, Upgrading Wood Gas Using Bentonite Clay: A Multiscale Modeling and Simulation Study, American Chemical Society Omega, 2020, 5, 11068.

M Lasich, Adsorption of H<sub>2</sub>S from Hydrocarbon Gas Using Doped Bentonite: A Molecular Simulation Study, American Chemical Society Omega, 2020, 5, 19877.

