PREVENTING OIL SPILLS CAUSED BY GAS HYDRATES

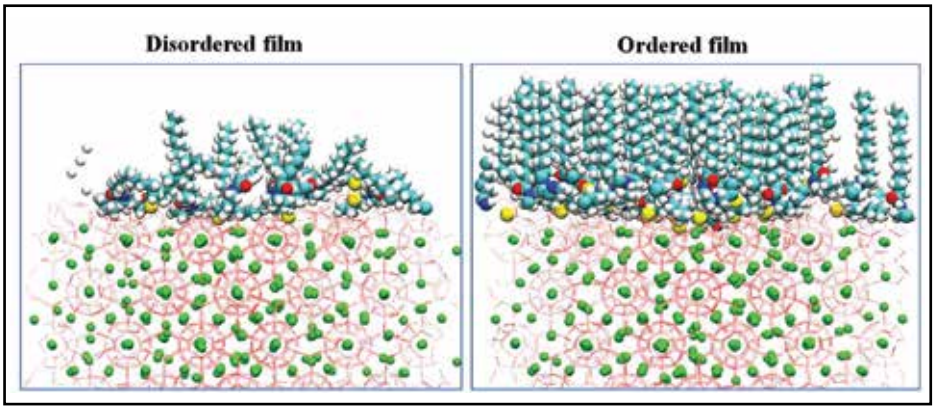
In the oil and gas industry, preventing spills is of the utmost importance. An oil or gas spill is not only damaging to the environment, but also costs significant amounts of money in lost product and clean-up.

Many oil and gas spills are caused when the pipeline fractures due to a blockage. Pressure builds up behind the blockage until the pipe eventually fractures. These blockages can be caused by gas hydrates. These are inclusions of water and gas molecules formed at low temperature and high pressure conditions. Gas hydrates are abundant in deep structures on the sea floor, and are considered a potential energy source and carbon storage method. However, they can stick together inside a pipeline, causing the blockage. Finding ways to stop these blockages from happening is very important.

At the moment, most pipelines use chemical hydrate inhibitors to reduce blockages. The most popular hydrate inhibitor is methanol, a thermodynamics inhibitor (TI) with ability prevent hydrate formation. However, this isn't ideal as a large amount of the inhibitor – up to 50% of the total water volume in pipeline - is needed to be effective. The inhibitor also needs to be injected directly into the pipeline, which is very expensive. The oil and gas spends hundreds of million dollars every year on injecting TIs in the pipelines to reduce the formation of gas hydrates. Alternatives are needed to reduce the cost and increase the efficiency of blockage prevention.

Another type of compound, called an anti-agglomerant (AA), could be used instead. AAs are chemicals that prevent hydrate particles from sticking together, so fluids inside the pipeline continue to flow. These chemicals can be effective at much lower volumes than traditional hydrate inhibitors, so would be much cheaper to use.

Research using ARCHER has helped us to understand the mechanisms responsible for the performance of anti-agglomerants. We have used ARCHER to conduct simulations, to discover how the structure of AAs contributes to their properties. The results will help develop new effective inhibitors for oil & gas pipelines.



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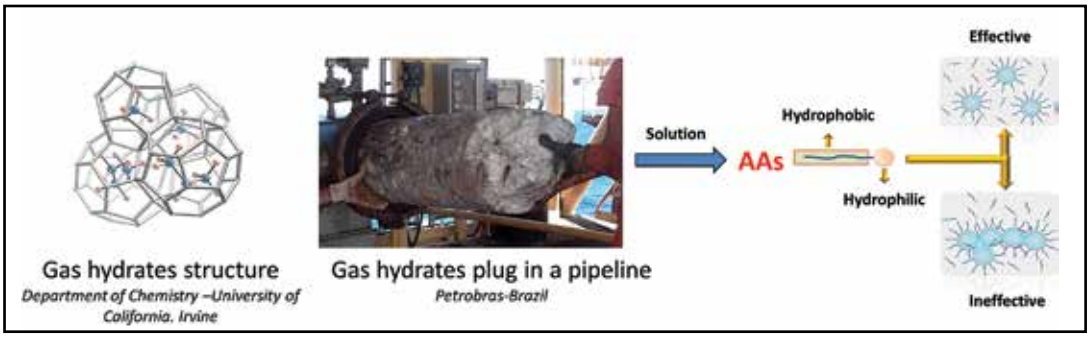

Researchers used ARCHER to understand the mechanisms responsible for the performance of anti-agglomerants, especially the contribution of the molecular structure of AAs, by using molecular simulations together with experimental works. The results will help develop new effective inhibitors as well as technologies to both harvest natural gas hydrates and engineer carbon dioxide hydrates for long-term storage applications.

Taking advantage of a powerful computational platform such as ARCHER was key, as the simulations were very complex. Molecular Dynamics simulations allowed the researchers to investigate how AAs behave at the hydrate-oil interface. These simulations provided new insights into properties of the layers in hydrate systems. This could not have been done experimentally, due to the complexity involved. It was found that some AAs form dense ordered films, from which methane molecules are excluded. The dense ordered films are believed to play a crucial role in preventing hydrate agglomeration.

To prove the results, the researchers conducted other simulations to quantify the energy barriers encountered when a water droplet and a methane molecule are transported towards the hydrate surface. The results revealed that the ordered AAs thin film creates much higher energy barriers compared to the ones formed by the disordered film. While experimental verification is needed, these findings could be used to design new types of AAs with better anti-agglomeration performance. There is also the potential to use this research for further applications in hydrate harvesting and carbon dioxide storage applications.

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About ARCHER

ARCHER is the UK National Supercomputing Service. The service is provided to the UK research community by EPSRC, UoE HPCx Ltd and its subcontractors: EPCC and STFC's Daresbury Laboratory, and by Cray Inc. Laboratory.

The Computational Science and Engineering (CSE) partners provide expertise to support the UK research community in the use of ARCHER, and researchers can also apply for longer-term software development support through the Embedded CSE (eCSE) programme. The ARCHER CSE partners are EPSRC and EPCC at the University of Edinburgh.

The Case Study Series

The ARCHER service facilitates high quality science from a broad range of disciplines across EPSRC's and NERC's remits. The outcome is science that generates significant societal impact, improving health and overall quality of life in the UK and beyond. This science influences policy and impacts on the UK's economy.

This case study is one of a series designed to showcase this science. It has been produced as part of the ARCHER CSE service, supported by EPSRC research grant No EP/N006321/1.

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