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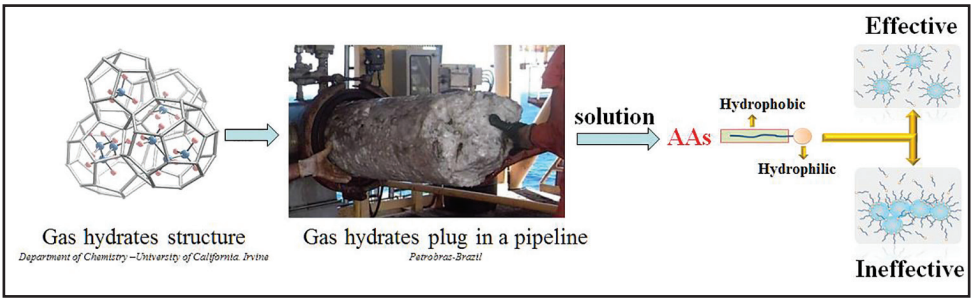
Tai Duc Bui is a third year PhD student at University College London. He is a student in the Department of Chemical Engineering studying interfacial phenomena in petroleum technology. He plans to use his prize to visit the Halliburton petroleum refinery in Texas, to take part in experiments to synthesise and test new anti-agglomerants.



My project focuses on preventing oil & gas pipeline blockages 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 structures on the sea floor, and are considered a potential energy source and carbon storage method. In the petroleum industry, however, gas hydrates can plug gas and oil pipelines. This causes the pipeline to fracture, spilling hydrocarbons out into the environment. As well as safety concerns, fractures will interrupt production and cause significant losses.

Currently, most operators use hydrate inhibitors such as methanol to reduce blockages. However, a large amount of the inhibitor (up to 50% of the pipeline volume) is needed to be effective. The inhibitor also needs to be injected directly into the pipeline, which is very expensive. 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 the pipeline continues to flow.

The goal of my project is to understand the mechanisms responsible for the performance of anti-agglomerants (AAs). 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.

Taking advantage of a powerful computational platform such as ARCHER was key, as the simulations are very complex. MD simulations allowed us to investigate how AAs behave at the hydrate-oil interface. These simulations provided new insights into properties of the layers in hydrate systems. We could not have done this experimentally, due to the complexity involved. We 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.