Quantum City

Quantum City Challenge

Applying quantum technology and solutions to Alberta's energy industry

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About the Quantum City Challenge

Quantum City is hosting an online challenge to demonstrate the ability to solve problems in Alberta's energy industry with quantum technology and/or solutions. Quantum City is working with Amazon Web Services (AWS) to facilitate this challenge and has received sponsorship from two Alberta-based energy organizations to demonstrate the applicability of quantum solutions for modern energy industry organizations.

Approach

We understand that quantum computing is a new technology and that currently available quantum computers are severely restricted by limitations on number of qubits, connectivity, error rates, and so on. The scale of the problem presented in this use case is far beyond what is possible for quantum computers today. The intention of this competition is to solicit new ideas of how to apply future quantum computers to solving such industrial (even if simplified) problems. For this reason, we welcome submissions including any of the below:

- Proof of concept solutions, on a smaller and perhaps simplified problem, including a formulation and/or implementation and/or resource estimates, solved on a currently available quantum simulator and/or actual quantum device.
- Hybrid quantum-classical solutions to the full problem or a subset of it, including formulation and/or implementation and/or resource estimates, solved using a currently available simulator and/or actual quantum device, or using a stand-in for a quantum computer to solve subproblems of a type that quantum computers might one day solve efficiently, such as SAT, MaxSAT, MIP, etc.

Purpose

Canadian Natural Resources Limited (CNRL) proposes the following problem statement for the Quantum City Challenge and welcomes novel quantum solutions for bitumen viscosity reduction.

Background

Canada contains the third largest crude oil reserves in the world. Canada's major oil production region is in Alberta, a province in the western part of the country. Oil is exported from Alberta via pipeline into other provinces in Canada and into the United States. Most of the oil in Alberta is heavy, either in the form of bitumen or classified as heavy crude.

The most cost-effective high-volume method of transporting crude via land is by pipeline and most Alberta oil moves on the existing pipeline network. Viscosity maxima and API gravity minima are specified by pipeline companies to ensure efficient operations and maximize movement of heavy oil from Alberta. Table 1 lists the current specifications for pipeline transportation, and the corresponding properties of bitumen.

Table 1: Pipeline specifications and bitumen corresponding properties.

Property	Specification	Athabasca bitumen	Diluted bitumen from in situ production[1]	Synthetic crude oil (SCO)[2]
Viscosity	maximum 350 centistokes (cSt) at pipeline temperature	5000 to 300,000 cSt at 25 °C	209 cSt at 15°C	8 cSt at 15°C
Density, kg/m³	< 940	1015	922.1±5.1	863.3±4.4
Gravity °API	>19	7.9	21.8±0.8	32.3±0.8
Bottom solids and water	< 0.5 vol%	0-2%	< 0.1%	0
Olefin content	< 1 wt%	0	0	0

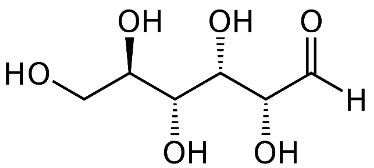
To satisfy these specifications, Alberta bitumen must be modified to meet pipeline specifications of viscosity and density. The predominant methods are:

1) Upgrading – This is where the bitumen molecule is cracked into lighter components under high heat and pressure and then blended into a synthetic crude. This is a capital-intensive process, but creates a more valuable crude. This also exceeds pipeline specifications.
2) Partial Upgrading – This is similar to upgrading, but utilizes a variety of methods to achieve results. This process is slightly less capital intensive than upgrading, but the aim of the process is to achieve pipeline specification or reduce the amount of diluent needed to achieve pipeline specification. There are no commercial applications of Partial Upgrading in Alberta at this time.
3) Dilution – Bitumen is diluted with a diluent, primarily light naphtha or natural gas condensate, to achieve pipeline specifications. When blended, it is called dilbit. About half of Alberta bitumen production is moved with the addition of diluent.
4) Viscosity Reducers – There are chemical compounds which modify the bitumen structure such that intermolecular forces are modified or reduced and allow the molecules to more easily 'slip' past one another. An example of a viscosity reducer is Octadecyl acrylate-maleic acid.
5) Mechanical Treatment – Mechanical treatment such as implementing ultrasonic energy can be used to break bonds in the bitumen molecule.
6) Higher Temperature – heating the bitumen to a higher temperature will reduce its viscosity and density.

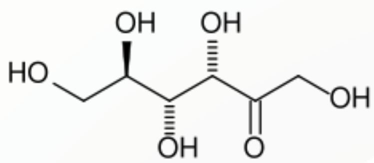
What is viscosity?

A liquid has the ability to flow because its molecules can slide around each other. The resistance to such flow is called the **viscosity**. Liquids which flow very slowly, like glycerin or honey, have high viscosities. Those like ether or gasoline which flow very readily have low viscosities.

Viscosity is governed by the strength of intermolecular forces and especially by the shapes of the molecules of a liquid. Liquids whose molecules are polar or can form hydrogen bonds are usually more viscous than similar nonpolar substances. Honey, mostly glucose ($C_6H_{12}O_6$) and fructose ($C_6H_{12}O_6$) is a good example of a liquid which owes its viscosity to hydrogen bonding.



Glucose



Fructose

Liquids containing long molecules are invariably very viscous. This is because the molecular chains get tangled up—in order for the liquid to flow, the molecules must first unravel. Fuel oil, lubricating grease, and other long-chain alkane molecules are quite viscous for this reason. Glycerol, $CH_2OHCHOHCH_2OH$, is viscous partly because of the length of the chain but also because of the extensive possibilities for hydrogen bonding between the molecules.

The viscosity of a liquid always decreases as temperature increases. As the molecules acquire more energy, they can escape from their mutual attraction more readily. Long-chain molecules can also wriggle around more freely at higher temperatures and hence disentangle more quickly.

Bitumen

Bitumen is a dense, highly viscous, petroleum-based hydrocarbon. In its natural state, bitumen can be a sticky, black liquid or an apparently solid mass that behaves as a liquid over very large time scales. At room temperature, it looks like cold molasses and must be either heated or diluted before it flows.

Bitumen is a complex substance with a diverse chemical composition. Its components are classified into four classes of compounds: saturates (saturated hydrocarbons), naphthenic aromatics (partially hydrogenated polycyclic aromatic compounds), polar aromatics (high molecular weight phenols and carboxylic acids), and asphaltenes (high molecular weight phenols and heterocyclic compounds).

The composition and properties of Athabasca bitumen can be found in Table 2. Molecular weight wise, bitumen is a mixture of about 300 - 2000 chemical components, with an average of around 500 - 700.

Table 2: Composition and properties of Athabasca bitumen.

Component	Units	Value
Carbon	wt%	83.1
Hydrogen	wt%	10.6
Sulfur	wt%	4.8
Nitrogen	wt%	0.4
Vanadium	wt ppm	145
Nickel, ppm by weight	wt ppm	75
Density	kg/m^3	1015
Gravity	API	7.9
Viscosity at 25 °C	cP or mPa s	300,000
Boiling fractions		
Light gas oil (LGO, 177 - 343 °C)	wt%	10
Heavy gas oil (HGO, 343 - 524 °C)	wt%	40
Vacuum residue, 524 °C +	wt%	50
Microcarbon residue (MCR)	wt%	13.6
Asphaltene, heptane (C_7) insoluble	wt%	11.5
Asphaltene, pentane (C_5) insoluble	wt%	17.2

Bitumen Viscosity

Heavy oil and bitumen macromolecules with branched planar fused rings and heteroatoms make it easy for molecules to produce non-covalent bonds and aggregate with each other. Among these non-covalent bonds, the hydrogen bond has the strongest binding ability. Heavy oil macromolecules increase the viscosity of heavy oil through the interaction of hydrogen bonds. Viscosity reducer molecules penetrate between asphaltene and resin flame molecules and combine with heavy oil macromolecules through strong electronegativity to form new hydrogen bonds, which prevent the aggregation of asphaltenes, resins and other macromolecules and make them disperse evenly and thus reduce the viscosity of the system.

Characterizing bitumen viscosity at room temperature is extremely difficult using typical lab procedures, making the trial-and-error approach to testing new viscosity-reducing reagents difficult:

- Specific experiments are difficult to perform at room temperature due to instrumentation and material limitations

- Experimental errors resulting from the difference in material and instrumentation factors cannot be avoided
- Lab methods are expensive and time consuming
- Molecular-scale underlying mechanisms are still unclear

Current Dilution Practice

Current practice to achieve pipeline specification is to mix bitumen with natural gas condensate or naphtha. Though toluene ($C_6H_5C_3$) is the most efficient solvent, its cost and availability make it unusable on an economic basis. Therefore, solvents of higher complexity or molecular weight, or viscosity-reducing molecules effective at lower dosages are required.

Examples of diluents can be found at CrudeMonitor. An example of a condensate blend can be found here.

Potential Quantum Approaches

There have been many attempts to identify and characterize bitumen viscosity and the role it plays at the molecular level.

A) Molecular Dynamic Simulations have been carried out to simplify the bitumen molecule into a variety of component models. These are classified anywhere from a 3 to a 20-component model of SARA (Saturates, Aromatics, Resins, Asphaltenes). Since the mobility of bitumen molecules is determined by the interactions between various molecules, the component models are then modeled using a variety of different forcefield models. The energy of one simulation consists of kinetic and potential energies, and a forcefield can be used to describe the intermolecular force between different atoms and molecules. There are many different forcefields that can be employed, but a common one is Condenses-phase Optimized Molecular Potential for Atomic Simulation Studies (COMPASS) and is implemented in LAMMPS. There are others and you should not feel limited to any particular one.

   Ren et al. (2022) provides an excellent summary document on the use of molecular dynamics simulation techniques to model the bitumen model. Zhang et al. (2022) demonstrates the use of both viscosity reducers and mechanical energy input, while running analyses using molecular dynamics simulation using a 4 component SARA model.

B) Machine learning on macro aspects of bitumen fluid systems can give insight into the classes of molecules that may be present, though the datasets are quite small, and in some cases the impact of temperature overshadows all other aspects of the system. One way in which these findings could be used is to verify outputs from quantum modeling. Please see the attached dataset. See Liu et al. (2023), and Khan et al. (2024)

C) Quantum methods have been applied to this problem, though they are often combined with molecular dynamics simulation. It is assumed that the asphaltene compounds interacting with one another are what is causing the high viscosity. Modeling using quantum methods focuses on reducing the total energy of the interaction, in particular van der Waals and electrostatic effects. Xu et al. (2022) have done interesting work in this area.

Solution Requirements

Beyond the information provided, we intentionally leave the solution requirements open, to allow contestants maximum room to show their creativity.

Baseline performance

The baseline is a 35% diluent to bitumen ratio, to meet pipeline specification of a viscosity of 350 cSt at 18°C and density 925 kg/m^3.

Data Sources

See attachment, and refer to the PhD Thesis by Motahhari (2013) for more information.

Detailed Problem Statement

Current practice to achieve pipeline specification is to mix bitumen with a diluent (natural gas condensate or naphtha) in a ratio of approximately 30% diluent to bitumen. This diluent is then recovered at the refinery or midstream where temperatures allow, and is sent back to the bitumen source. The use of condensate carries a cost, and takes up pipeline capacity, which increases energy requirements to move this fluid back and forth within the pipeline network. Therefore, solvents of a different configuration or viscosity-reducing molecules that can lower the ratio of diluent to bitumen are desired.

Since bitumen is a complex molecule, it is difficult to predict viscosity on a macro scale by looking at the bitumen molecule at the nano scale. It is of interest to gain insights into the bitumen molecule and build a viscosity model based on bitumen composition, molecule addition and temperature, but from the quantum/molecular level.

Furthermore, it is also of interest is to identify viscosity-reducing molecules that will either take up hydrogen bonding sites on the asphaltene and resin compounds to prevent intermolecular attraction or reduce the van der Waals interaction between molecules.

Constraints

Temperature is the most obvious and effective way to reduce bitumen viscosity. However, doing so on an industrial scale is both capital and energy intensive. We are looking for solutions using means that are chemistry based, rather than ones where the main component is the manipulation of temperature.

Metals should not be included as part of the solution, unless they fit into product specifications. As an example, WTI (West Texas Intermediate) crude specifications limit nickel to 8 parts per million or less by mass and vanadium to 15 ppm or less by mass (see CME website, for example).

Reduction of viscosity can be achieved by precipitating heavier components of the bitumen molecule, in particular asphaltenes. However, pipeline specifications require that no material is precipitated and deposited in the pipeline during operation. Therefore, solutions that rely on precipitation to reduce viscosity reduction in pipeline will not be considered.

References

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