Quantum City Challenge

Applying quantum technology and solutions to Alberta’s energy industry

Quantum City

Canadian Natural

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 tailings surface charge consolidation.

Background

In Fort McMurray, oilsand ore is mined and processed to extract bitumen and convert it to synthetic crude oil. More than 1.4 million barrels of bitumen are produced daily from different mining facilities. The process of oilsand mining involves removing overburden and vegetation, mining the oilsand ore, extracting the bitumen from the oilsand, returning the mineral (sand) back to position in the form of tailings, treating the tailings, and reclaiming the previously mined areas by replacing overburden and vegetation.

Oilsand ore is made up of bitumen, water, and minerals (See Table 1)[i].

Table 1: Oilsand mineral components.

Component	Weight percent
Sand	82
K-feldspar	5
Calcite	Trace
Dolomite	Nil
Siderite	Trace
Pyrite	Nil
Kaolinite	4
Illite	7
Chlorite	1
Smectite/Montmorillonite	Trace
Mixed layer clays	1
Anhydrite	Trace

To separate the bitumen from the oilsand, the ore is mixed with hot water to create a slurry and is then pipelined over several kms. In the pipeline, the bitumen is liberated from the mineral through thermal energy, and attaches to entrained air bubbles, while the mineral breaks down through mechanical agitation into smaller and smaller particles.

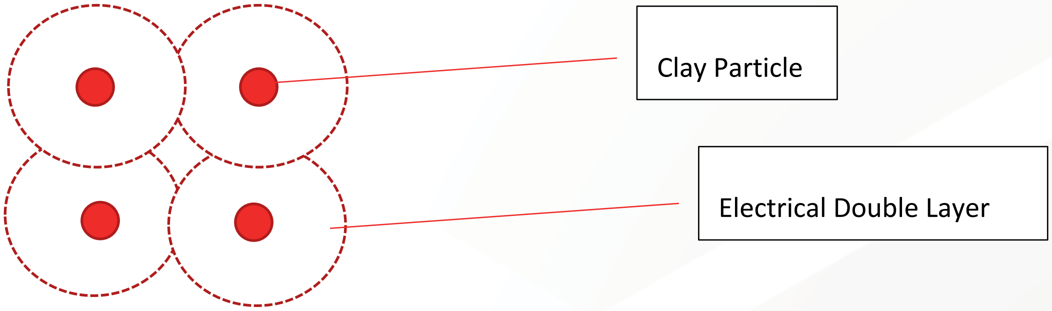
The slurry enters a separation process where the aerated bitumen floats to the top, while the mineral slurry settles and is pumped to a tailings pond. This mineral slurry is called tailings, and is made of a collection of sand, clays and other trace minerals.

If left untreated, the tailings will settle into layers of fluid fine tailings (FFT), water, and sand. It is this fluid fine tailings layer that is the focus of this challenge. FFT is a clay dominated slurry that encompasses clay, entrained sand (silica) and water. The clay particles will exhibit a surface charge in water.

Clay

Clay particles are extremely small (less than 0.002 mm in size) and will not settle readily, if at all, even in still water. The small size of these particles means that they have an extremely high surface area relative to the volume of the particle. When negatively charged clay particles are suspended in water, they tend to repulse each other, much the same way similar poles of magnets repel each other. The cumulative effect of the repulsion of a vast number of small particles prevents their aggregation into larger, heavier particles that would settle more readily[ii].

These clay particles also attract water and water is adsorbed onto the surface of the clay particle. The adsorbed water directly affects the surface charge density of the clay particle through an effect called the electrical double layer. This creates a type of field around the particle that prevents these clay particles from agglomerating together. The clay surface is in direct contact with this rigid layer of water molecules that depending on the charge density and specifically adsorbed cations extends over two additional layers of water molecules. Beyond this layer is a diffuse space charge distribution that shields the excess charge of the inner layers.



This prevents a challenge for mine site remediation, since this layer of FFT will not be reclaimable without intervention. The clays in the FFT layer will consolidate until they reach an equilibrium of approximately 30% mineral by weight. This layer will exhibit a yield stress and will be able to suspend other particles, though will not gain enough strength required to build reclamation soils on top (modelled to be approximately 15 kPa).

There are four types of clays that occur in bitumen extraction from oilsands tailings (see Table 2). They are kaolinite, illite, montmorillonite and chlorite.[iii] While kaolinite is the highest clay in abundance, it is illite and montmorillonite which present the greatest challenge. The reason being that their high specific surface area and high cation exchange capacity makes them particularly difficult to capture and settle without the use of mechanical aids. Furthermore, when dispersed in water, clay particles have a high affinity for water and readily swell.

Table 2: Clay type and their characteristics.

Mineral	Kaolinte	Illite	Montmorillonite	Chlorite
Abundance (wt. %)	69	28	0.3	1
Composition	$Al_2Si_2O_5(OH)_4$	$K(Al,Fe,MG)_5(Al,Si)_8O_{20}(OH)_4$	$(Na,CA,H_3O)_x[Al_{4-x}(Fe,Mg)_xSi_8O_{20}(OH)_4]$	$(Mg,Fe,Al)_6(Al,Si)_4O_{10}(OH)_8$
Type of Structure	Two-Layer (TO)	Three-Layer (TOT)		
Cleave (Basal planes	SiOSi silixane Al-OH hydroxyl	SiOSi siloxane		SiOSi silixane MgOH hydroxyl
Isomorphic Substitution	Low in T	High in T	Both in T and O	
Compensating ions	K^+	K^+	Na^+, Ca^{2+}	O-brucite
Specific surface area (m2/g)	10-20	65-100	50-120 (external) 700-840 (total)	42
Cation exchange capacity (meq/100 g)	3-5	10-40	80-150	10-40

Current Treatment Practice

Current practice to treat tailings is to agglomerate the clays is to use coagulation and flocculation, with perhaps some form of mechanical energy applied. Flocculation is a process of contact and adhesion whereby dispersed particles form larger-size clusters. Flocculation can occur through the use of a coagulant, flocculant or both. Coagulants achieve flocculation through charge neutralization whereas flocculants physically bind clay colloidal particles together.

A coagulant contains positive ions (typically as sodium, calcium or aluminum in inorganic variants or amine in organic variants) that neutralizes or destabilizes the negative charges on the clay particles. Coagulants assist dewatering in part by specifically adsorbing onto the clay surface along the plane of vicinal water molecules. Higher valence cations with greater charge are more effective for charge neutralization. However, a high dosage of coagulants causes the free water to be hard. When recycled to the extraction plant they impede natural surfactant release that is essential for bitumen extraction. Also, coagulants can be toxic to aquatic environment, thus impeding reclamation.

Flocculants, on the other hand are natural or synthetic polymers used to generate stable flocs that are networks with clay particles attached to the polymers structure. Flocculants provide counter ions that reduce the repulsive forces between clays so that they can rearrange and form flocs as well as bridge flocs together to form aggregates. Some water remains trapped within the network and require mechanical shear or other external force to be released. However, the shear breaks down the network structure and may result in reduced settling. The charge density, molecular weight and the overall chemical properties of the polymer control its hydrophilic (absorbs) or hydrophobic (repels) binding interactions with the clays. These interactions play a significant role in flocculant efficacy and subsequent solids separation and management. Flocculants can be used alone, or in combination with coagulants.

The efficacy of the coagulant and flocculant for tailings treatment is dependent on many factors such as water chemistry and properties (pH, temperature, ionic strength, dissolved salts concentration and composition, and turbidity, etc.) and the sequence of addition and dosage of these chemicals. However, even with the best practice developed from experience the approach had not been entirely successful. Part of the challenge is that these chemical additives only modify the electric field of the clay and enable better rearrangement of the solids but do not drive away (squeeze) the rigid water associated with the clay particles, resulting in limited dewatering. Also, the interactions between different phyllosilicates with these chemicals added in different sequences in a complex environment are yet not well-understood. This is the key to successful tailings treatment method based on chemical amendment.

Complicating things further, all of the water recovered in tailings is reused in the bitumen recovery process, which has its own challenges related to clay activity and water chemistry. Thus, the use of coagulants is challenging and is thus limited in scope.

Solution Requirements

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

Baseline performance

Dosing flocculants at 1000 g/t of solids allows clay to settle to approximately 55% solids/w without mechanical intervention or blending with sand. At 1 m^3 of slurry, 30% solids, density of 1.3, would mean that you dose at 1 m^3 slurry * 1.3 density * 30% solids * 1000 g/t = 390 g of flocculant.

Detailed Problem Statement

Current practice to agglomerate clay particles is expensive and can be energy intensive. Mechanical intervention approaches have included the use of thickeners, filter presses, centrifuges etc. The best approaches to date have been to treat the clay particles with a coagulant and an anionic flocculant and then mix the solution with a coarse sand slurry to create a sand/clay deposit with sufficient yield stress to withstand the forces of heavy equipment. Typical sand to clay ratios of mixing are on the order of 4:1.

Gypsum ($CaSO_4\cdot 2H_2O$) and Alum ($XAl_2\cdot 12H_2O$) have been considered as coagulants in the process of treating tailings though their use is not widespread, due to issues identified earlier. When they have been tested in the laboratory, they have shown to be effective at reducing the surface charge of clays.

Polyacrylamides are the most widely used anionic flocculants for tailings and water treatment purposes. While they are effective at binding clay particles together, they do not overcome the electric double layer of the clay surface and are thus limited in how much they can agglomerate clay particles, without the use of sand mixing or mechanical intervention.

It is desired to find a coagulant/flocculant formulation that will reduce the electric double layer of the clay particle and bind the clay particles together such that they can be agglomerated into a solid concentration greater than 70%/w, and with a lower sand to clay ratio (less than 3:1). Treatments that exhibit low toxicity in their application would be appreciated. Natural flocculants such as chitosan, starch, cellulose, and gelatin may be unique treatments that have not been explored in depth.[iv]

References

[i] Masliyah et al., Handbook on Theory and Practice of Bitumen Recovery from Athabasca Oil Sands. 2011; https://doi.org/10.7939/r3-nr43-8t34

[ii] Chemical coagulants and flocculants – Sediment Control Technique; https://www.austieca.com.au/documents/item/818

[iii] Masliyah et al., Handbook on Theory and Practice of Bitumen Recovery from Athabasca Oil Sands. 2011; https://doi.org/10.7939/r3-nr43-8t34

[iv] El-Gaayda et al., Natural flocculants for the treatment of wastewaters containing dyes or heavy metals: A state-of-the-art review; Journal of Environmental Chemical Engineering 9 (2021) 106060; https://doi.org/10.1016/j.jece.2021.106060