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Sediment Diagenesis Module for CE-QUAL-W2. Part 1: Conceptual Formulation

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Abstract This paper presents a conceptual framework for a sediment diagenesis model that was developed as an add-on module to the hydrodynamic and water quality model CE-QUAL-W2. The module was designed for oil sand pit lakes, but has been developed such that it is applicable to other waterbodies, particularly those with subaqueously placed mine waste or organic-rich sediments. The module includes important physical and chemical processes such as the following: tailing consolidation coupled with lake bed deepening and pore-water release, biogenic gas production (build-up and release of methane, hydrogen sulfide and ammonia), bubble release through the water column, unconsolidated sediment resuspension during bubble ebullition, dynamic oxygen consumption at the sediment-water interface and in the water column from bubbles, and salt rejection during ice formation.

Keywords Athabasca oil sands · End pit lakes · Mature fine tailings · Methane · Diagenesis · Gas release · Bubbling · Bed consolidation · Oil sands

This is a two-part paper, along with *Sediment Diagenesis Module for CE-QUAL-W2 Part 2: Numerical Formulation*

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1 Introduction

This paper presents a sediment diagenesis module that was written as an add-on to the hydrodynamic and water quality model CE-QUAL-W2 (*C*orps of *E*ngineers, water *QUAL*ity model for *W*aterbodies of *2*-dimensions). The module was originally developed for predicting the physical and chemical behavior of submerged tailings in pit lakes developed as closure waterbodies for the oil sand industry. Both the conceptual formulations presented herein, and numerical formulations presented in Prakash et al. [21] of the module, however, were based on generic diagenesis processes that are applicable to other waterbodies, particularly lakes with submerged tailings or lakes that have sediments with high organic content, whether natural or contaminated. The module can also predict greenhouse gas emissions from such systems.

1.1 Background

The oil sands of Alberta, Canada, contain approximately 170 billion barrels of proven oil reserves. In the Athabasca Oil Sands Region, north of Fort McMurray, the highly viscous hydrocarbon resource, bitumen, is near the surface and sufficiently concentrated to be recovered using conventional surface mining and chemical extraction. Presently, six surface mining projects are operating in the Athabasca Oil Sands Region; other projects are at various stages of the regulatory approval process.

Similar to most mining operations, oil sand mines include pit lakes in their closure and reclamation plans. Approximately 35 pit lakes are proposed for the region (Fig. 1). About half of these will have permits that specify that Mature Fine Tailings (MFT) be placed in the pit before the pit is flooded with fresh water to create a pit lake.

MFT is a mixture of fine clay materials that settle much more slowly than the coarser tailings [18] and therefore pose

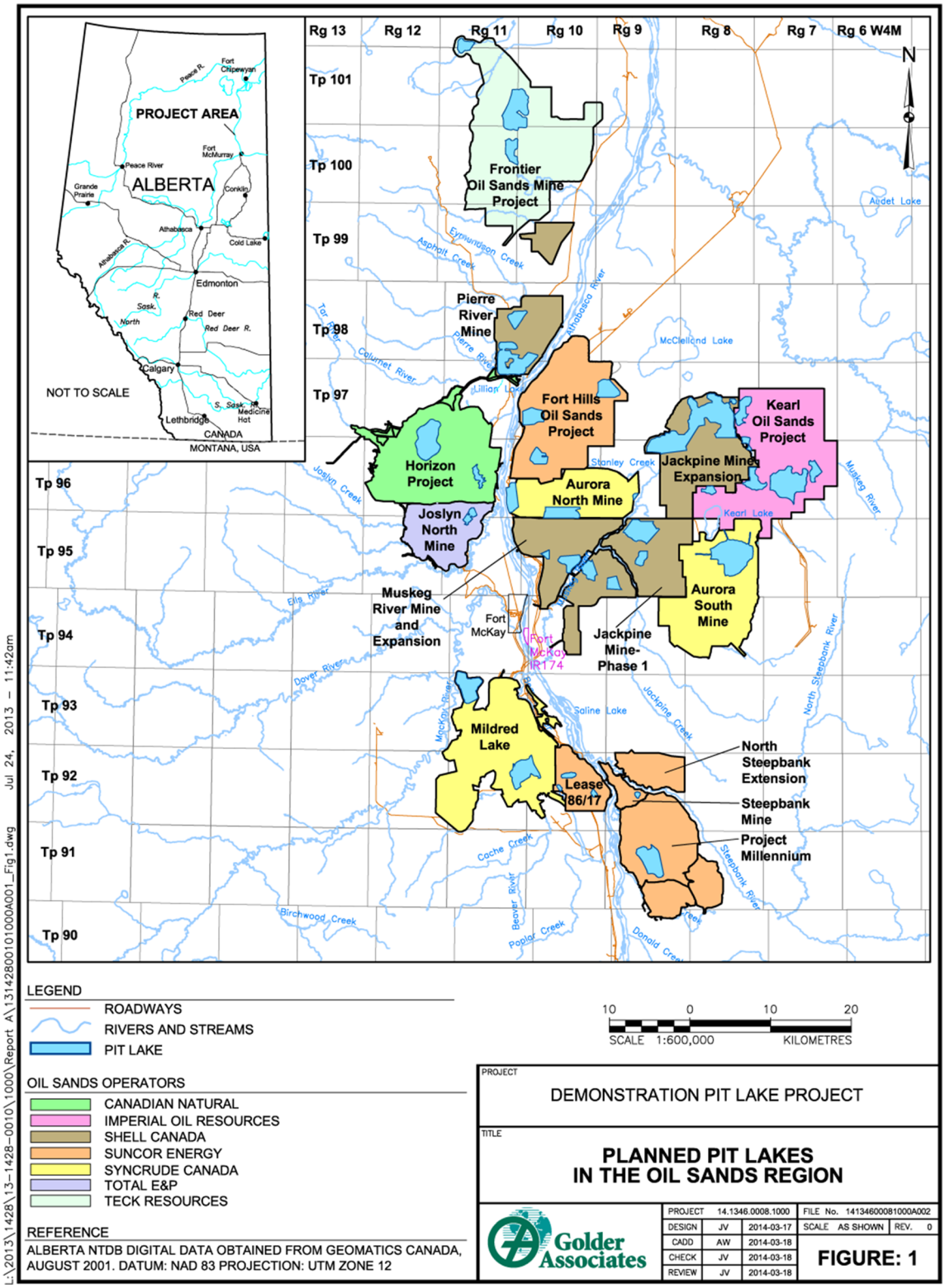

Fig. 1 Planned pit lakes in the Oil Sands Region

challenges to reclamation. Oil sand tailings contain residual organic compounds such as naphthenic acids, phenolics and polycyclic aromatic hydrocarbons [14, 15, 18, 24], which must be contained or degraded prior to release of pit lake water to the surrounding environment. At present, all oil sand mines operate as closed-circuit systems, with the exception of one facility that maintains a licensed discharge from an associated bitumen upgrader. Each pit lake will be maintained

within the closed-circuit system until the water quality in that lake is certified by regulatory authorities as acceptable for release.

As part of the application for regulatory approval of an oil sand mine, pit lake performance is evaluated for the environmental impact assessment using various models to predict water quality in each pit lake and in receiving watercourses (e.g., [23]). While these models incorporate the effects of water released from MFT using assumptions regarding the quality of MFT release waters, there are currently no models available to (1) simulate the relevant processes that occur within the MFT and estimate pore-water quality, (2) simulate the formation and release of gas bubbles, and (3) simulate the physical and chemical interaction of gas bubbles in the water column.

1.2 Study Objectives

The objective of this study was the development of a sediment diagenesis module that mechanistically addresses the limitations of the current set of models and which is incorporated into Version 3.6 of the CE-QUAL-W2 computational framework. These processes include physical, chemical, and biogeochemical reactions within MFT that may result in the release of aqueous and gaseous compounds into the water column. The model simulates anaerobic decay of these compounds and production of gasses such as methane, carbon dioxide, and hydrogen sulfide.

The study used a stepwise, research-based approach: relevant algorithms were identified, a computational framework was developed to accommodate the algorithms, and the system was coded and tested. Datasets necessary to refine the algorithms by comparing computed with observed values of key parameters are currently limited. When planned data collection efforts are complete, the model formulations will be validated and the model will be refined so that it can be used for full-scale systems. The model is open source and available on request at www.gemss.com/W2SedDiagenesis/W2SedDiagenesis.htm.

1.3 Model Platform

CE-QUAL-W2 is a longitudinal-vertical hydrodynamic and transport model built for long-term, time-varying water quality simulations of rivers, lakes, reservoirs, and estuaries. CE-QUAL-W2 reproduces vertical and longitudinal water quality gradients and is capable of multi-decade simulations. The model is described in Buchak and Edinger [5], Cole and Buchak [6], and Cole and Wells [7]. These publications present formulations of the fundamental equations, the structure of the computations, and summaries of applications. Source code, user manuals, documentation, and applications to specific waterbodies for CE-QUAL-W2 are available at http://www.ce.pdx.edu/w2/. The user manual lists multiple validation exercises and quantifies goodness-of-fit. The website presently lists approximately 2400 worldwide applications of the model to water quality problems.

Of interest to oil sand pit lakes is the ability of the model to make use of historical and projected climatic data to extend the simulations to multiple decades, the expected period which will be required for pit lakes to produce water suitable for release. Williams [30, 31] validated his CE-QUAL-W2 model application to Lake Powell, a large lake in the American Southwest used for water supply and hydropower, by making a single CE-QUAL-W2 simulation that covered 19 years. He subsequently compared modeled values with observations. The model consistently reproduced observations without deviations of computed and observed values growing over time.

2 Model Framework

At the initiation of the project, processes were identified as key drivers affecting pit lake water quality that were not available in existing models: tailings consolidation (which includes lake deepening and pore-water release); gas production (which includes the physical processes of bubble formation and ebullition); unconsolidated sediment resuspension and erosion; non-algal water clarity; fully coupled, dynamic oxygen demand from sediment, dissolved constituents, and bubbles; and salt rejection from ice formation. These processes are shown conceptually in Fig. 2 and discussed in more detail below.

2.1 Tailing Consolidation, Lake Deepening, and Pore-Water Release

Tailings placed in oil sand pit lakes will consolidate over time, releasing pore water into the water column. The overall effect is that the pit lakes will deepen over time. The time for complete settling of MFT has been estimated at 125 to 150 years [9], although methanogenesis and other biochemical reactions may reduce this settling time considerably [11, 12, 25].

CE-QUAL-W2 is a traditional, fixed-grid model with a static bathymetric surface onto which longitudinal segments and vertical layers are mapped; the hydrodynamic and water quality computations are performed at the intersections of these segments and layers. The bathymetry and, consequently, the gridded representation of the bathymetric surface are fixed throughout a simulation.

To include the process of tailing consolidation and the resulting lake deepening, modifications to the CE-QUAL-W2 code were made to include a time-varying

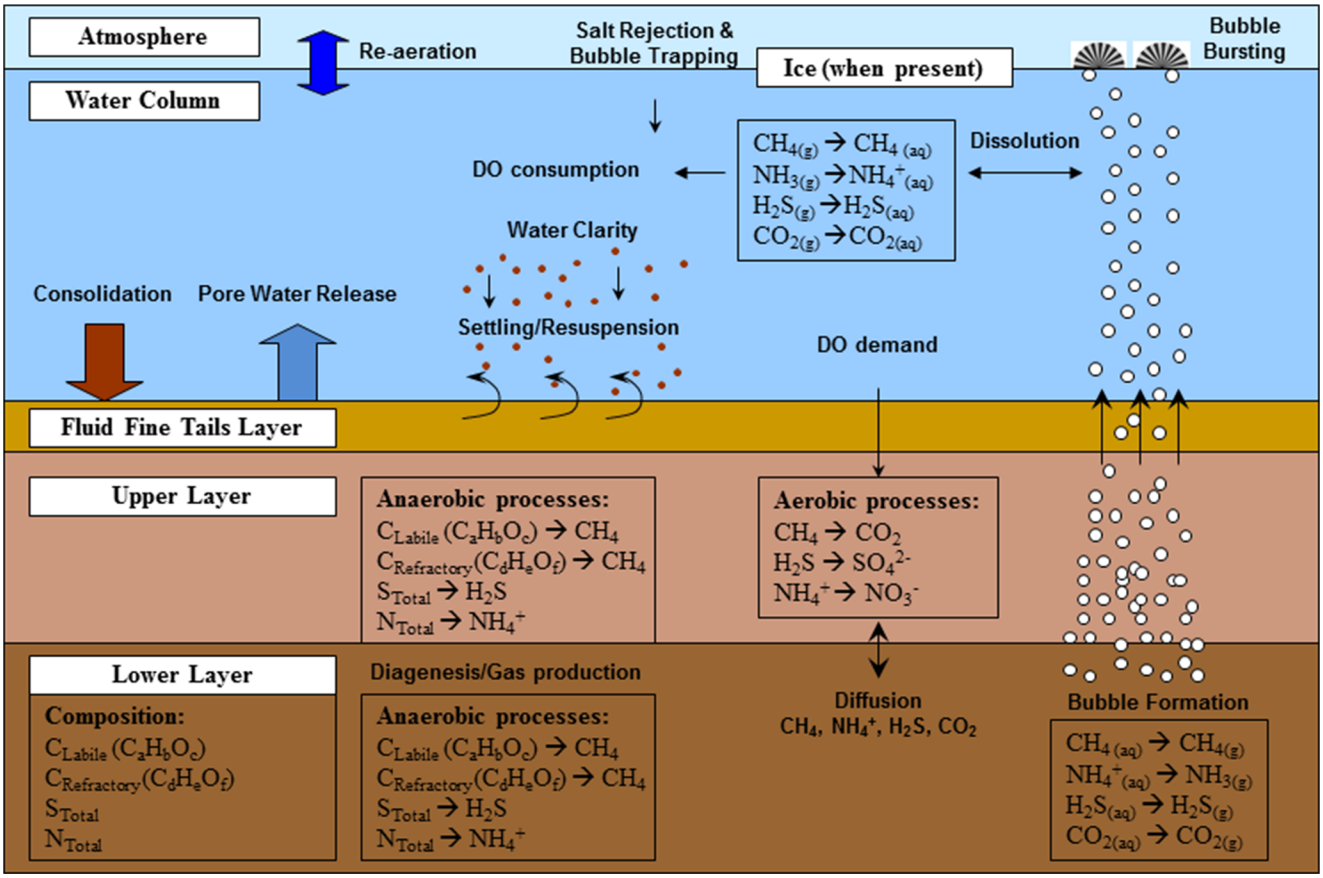

Fig. 2 Conceptual diagram of processes included in the oil sands pit lake model. Conceptual diagram illustrating major processes that have been added to the module. Tailing consolidation results in dynamic bed elevations and pore-water release; diagenesis and gas production within the upper and lower sediment layer results in bubble formation and ebullition; bubble release results in unconsolidated sediment resuspension and erosion; these processes affect water clarity and are coupled to dynamic oxygen at the sediment interface and in the water column; and bubbles are trapped and salts are rejected during ice formation. A fluid fine tail layer overlies the sediment layers

lake bottom. As modified, the model grid is developed from the initial lake bathymetry. During a simulation, the tailings consolidation is calculated based on user-defined rates that can vary spatially for each segment. Consolidation rates are not calculated by the module, but can be derived through separate models, such as a finite strain or empirical model [4, 9, 29, 33], then entered into the module. In each segment, a new bed elevation is calculated at each computational time step and compared to the initial bed elevation. When the difference in the changed bed elevation and original bed elevation reaches a user-defined fraction of the bottom grid layer thickness, a new grid layer is added.

During consolidation, tailing bed porosity and total pore volume are calculated based on the consolidation rate. A volume of pore water, equal to the change in total pore volume since the previous timestep, is expressed from the tailings. This pore-water volume is released into the overlying water column along with the pore-water constituents listed in part 2 of this paper [21].

2.2 Tailing Gas Production

The gas production module includes three basic processes. The first process is diagenesis (or decay) of organic matter that consists of particulate organic carbon (POC), particulate organic nitrogen (PON), and sulfate. Both PON and POC are further subdivided into labile, refractory, and inert reaction classes based on diagenesis rates. The labile class represents rapidly decaying organic matter, the refractory class represents slow decaying organic matter, and the inert class represents any fraction of PON or POC that does not participate in the diagenesis process. Inclusion of the inert class is required for the mass balance of the system.

The second basic process is the flux of substances produced by diagenetic processes to the upper, aerobic layer and to the water column. The third basic process is oxidation in the aerobic layer which consumes oxygen diffused from the water column, exerting sediment oxygen demand (SOD) on the overlying water.

The module uses DiToro's [8] two-layer sediment diagenesis formulation as the computational basis. This formulation employs an upper layer, which can be either aerobic or anaerobic, depending on the oxygen balance of the system, and a bottom layer that is always assumed to be anaerobic. The upper layer has a varying depth depending on oxygen penetration from the overlying water column. The presence or absence of oxygen in the upper layer controls all oxidation processes in this layer. When oxygen is absent in this layer, anaerobic processes may occur. Even at its maximum thickness, the upper layer is a small fraction of the total sediment bed in terms of volume. The anaerobic lower layer is the predominant source of diagenetic fluxes.

The sediment bed is thus represented by two homogeneous sediment layers, an assumption which is a possible limitation that will be refined if the model cannot be calibrated to real systems. A third layer, the fluid fine tail layer, is a model layer within the water column of CE-QUAL-W2 that contains very high (up to 30 %) solids by weight. It is added as an insulating layer above the sediment module to reflect the transition between sediment and water.

2.3 Mass Balance Equations

The equations developed for the model rely on the principle of mass balance. The equations shown in this report assume a limitless supply of water and protons, so these are omitted from the chemical reactions and mass balances.

The mass balance equations for the two-layer model for a constituent C are shown in Eqs. 1 and 2.

(Upper layer)

$$H_1\frac{dC_1}{dt} = J_1 + K_{L12}(C_2 - C_1) + K_{L01}(C_0 - C_1) - K_{r1}C_1 \quad (1)$$

(Lower layer)

$$H_2\frac{dC_2}{dt} = J_2 + K_{L12}(C_1 - C_2) - K_{r2}C_2 \quad (2)$$

where H is the layer thickness, J is the production (source) flux, and K is the decay/reaction loss for constituent C. Time is shown as t. Subscripts 1 and 2 denote the values for upper and lower layers, respectively. K_{L12} is the mass transfer (diffusion) coefficient between the layers. C_0 is the concentration in the overlying water column, and K_{L01} is the mass transfer coefficient between the upper layer and the water column.

2.3.1 Nitrogen

PON in the sediment bed decreases in concentration as a consequence of mineralization to ammonia. Ammonia (NH_3) may be oxidized to nitrate (NO_3^-), but only in the upper layer when oxygen is available for the reaction. Ammonia also undergoes ionization (NH_3 to NH_4^+), depending on a user-specified pH of the pore water. Finally, ammonia may undergo dissolution ($NH_{3(g)}$ to $NH_{3(aq)}$) according to Henry's Law.

2.3.2 Carbon

Methane (CH_4) and carbon dioxide (CO_2) are produced by the anaerobic decay of POC involving a consortium of microbes. In the aerobic zone, methane can be oxidized by methanotrophic microbes to produce CO_2 and H_2O. Sulfate inhibition of methanogenesis has been found to occur when the sulfate concentration was above 20 mg/L [10]. Based on these observations, a user-specified, sulfate-inhibition concentration was added to the model, with a default value of 20 mg/L of sulfate. Below this value, methanogenesis may occur. Above this value, consumption of POC occurs while reacting with sulfate to form sulfide.

The rates of reactions applied in the diagenesis formulations are generally temperature dependent (Eq. 3).

$$k = k_r\theta^{(T-20)} \quad (3)$$

where k_r is the reaction rate, θ is the temperature coefficient, and T is the temperature.

Reaction rates in the diagenesis formulations applied in the module make use of this temperature-dependent relationship. The "Q_{10} effect," where the enzymatic activity approximately doubles with each 10 °C temperature rise, occurs with a temperature coefficient of 1.07. Temperature is computed by CE-QUAL-W2 and is readily available at each location through time.

2.4 Bubbling to Surface

Continuous production of dissolved gasses (H_2S, CH_4, CO_2, and NH_3) through diagenesis may result in oversaturation, at which point bubbles may form. The relationship between the dissolved and gaseous (bubble) phase is described by Henry's Law. In situ rates of bubble formation have not been measured in MFT, and thus the module relies on generic bubble formation and growth relationships. The growth model adopted for the module is based on the work of Boudreau et al. [2, 3]. This model was chosen because it considers a distributed source of gas formation which is not normally included in other bubble growth models. This approach is important as the sediment

bed continually produces gas through diagenesis. Boudreau et al. [2, 3] note that the validity of the model is restricted by its assumptions but that the results are correct within an order of magnitude, even if some of the assumptions are violated. A complete bubble creation and release model would include nucleation, kinetics of gas adsorption, gas transport, and mechanical response of the sediments. However, nucleation kinetic limitations are overcome by assuming that there are abundant nucleation sites and that the bubbles form without hindrance. Similarly, the rate of growth of bubbles in sediments is sufficiently slow that adsorption kinetics can be ignored. This assumption leaves only transport and mechanical controls to be considered.

The main assumptions in the algorithm for bubble growth and release include as follows:

- Gas bubbles are spherical.
- Gas bubbles are only released when cracks occur in the sediment bed.
- Cracks in the sediment bed close when bubble pressure drops below a fraction of crack formation pressure.

While studies have been carried out to understand bubble-induced turbulence, our knowledge is currently insufficient for the development of accurate models of the effects of bubbles on turbulence properties in bubbly flows [16]. A simplified correction that accounts for bubble-induced turbulence based on the turbulence viscosity [16] has been adopted for the module.

Once the bubbles are released into the water column, their rise velocity is determined by the buoyant forces acting on them. Due to the wide range of possible gas bubble sizes, the more general formulations of Zheng and Yapa [32] were adopted for use in the module. Although spherical bubbles are assumed in the module, the rise velocity computations from Zheng and Yapa [32] are also applicable to non-spherical bubbles.

2.5 Unconsolidated Sediment Resuspension and Erosion

In both tailings and natural bed materials, unconsolidated sediments can undergo resuspension into the water column. The resuspension process was added to the original CE-QUAL-W2 code based on common formulations used in sediment transport models.

Cohesive bed erosion occurs in two distinct modes: mass erosion and surface erosion [26]. Mass erosion occurs rapidly when the bed stress exerted by the flow exceeds the shear strength, τ_s, of the bed. In contrast, surface erosion occurs gradually when the flow-exerted bed stress is less than the bed shear strength but greater than a critical erosion or resuspension stress, τ_e, which is dependent on the shear strength and density of the bed. Typically, under accelerating flow resulting in increased bed stress, gradual surface erosion takes place first, followed by mass erosion. If the bed is well consolidated, then only surface erosion occurs.

The non-cohesive sediment particles that settle from the water column accumulate on the sediment bed. Under the influence of moving water and its shear exerted on these bed sediments, the particles experience an uplifting force which, if greater than critical shear stress for erosion, transports the particles back into the water column. The module quantifies the non-cohesive sediment erosion based on the formulation of van Rijn [28].

Erosion is modeled as the diffusive flux of sediments into the water column. This diffusive flux is computed based on estimating the bed sediment concentration and near-bed sediment concentration. The module estimates instantaneous bed elevation based on the mass balance that includes net deposition, resuspension, and tailing consolidation.

2.6 Non-algal Water Clarity

Water clarity or turbidity is an indicator of the amount of total suspended sediment (TSS) and organic material in the water column. Relationships between TSS and turbidity can be developed based on site-specific data. The statistical relationship between TSS and turbidity is taken to be linear on a natural logarithmic scale [19]. A generic relationship for the two entities in the module is given by Eq. 4:

$$\ln(\text{Turbidity}) = A_{\text{turb}} \ln(\text{TSS}) + B_{\text{turb}} \tag{4}$$

Both A_{turb} and B_{turb} are site-specific parameters. The TSS concentrations are calculated internally in the model and, based on the values of A_{turb} and B_{turb}, turbidity values are expressed in Nephelometric Turbidity Units (NTU).

2.7 Oxygen Dynamics

Pore water and gasses released from the gas production module exert additional SOD, which results in variable lake-bottom oxygen consumption. The module links oxygen demand from sediment and bubbles to the existing biochemical oxygen demand (BOD) routines in the CE-QUAL-W2 code. In the water column, gas dissolution is dictated by Henry's Law. Once dissolved, the ammonia exerts an oxygen demand during nitrification. A similar procedure is used to estimate oxygen consumption for other gasses including methane and hydrogen sulfide.

In the aerobic zone of the sediments and water column, methane will be oxidized if conditions are suited to methanotrophs. Methane oxidation has been found to occur in narrow bands within the thermocline due to the dependence of methanotrophs on an oxygen-sensitive

nitrogen fixation process [1, 13, 22, 27]. In these studies, most methane was oxidized at this oxic/anoxic interface. Following lake turnover, the methanotrophs were able to oxidize methane throughout the water column, which was attributed to ammonia entering the epilimnion from the hypolimnion. Once the ammonia had been consumed in the epilimnion, high oxygen concentrations precluded nitrogen fixation, which in turn precluded methane oxidation [22]. Other studies have found that the majority of methane oxidation occurs near the sediment-water interface in a narrow zone between the aerobic and anaerobic layers [13, 17]. While methanogens cannot function in aerobic conditions, they can tolerate oxygen stress for prolonged periods [20] and are therefore able to persist in zones with fluctuating oxic conditions.

In the water column, this process is modeled using the standard CE-QUAL-W2 formulation described in Cole and Wells [7]. In the sediment layer, generic BOD constituents are added in a similar fashion to how they are added and modeled in CE-QUAL-W2. As the generic BOD constituents are released from the sediment layer, they are internally linked to CE-QUAL-W2 and they exert a BOD in the water column. Naphthenic acids are an example of a generic BOD constituent that can be added to the sediments and water column in the module.

2.8 Salt Rejection

The rejection of salts during ice formation is a process that is not included in most standard ice modules, including the standard ice modules in CE-QUAL-W2. Salt rejection was added as a mechanistic process to the detailed ice module, without the need for external files. Salt rejection was included by removing 0.917 m^3 of water from the top layer for every 1 m^3 of ice formed to account for differences in density.

The ice module was also configured to trap bubbles under the ice. During the ice-cover period (as predicted by the detailed ice-cover module), bubbles are not allowed to escape and remain effectively bound at the upper surface of the water column where they can interact with aqueous constituents. Once the ice melts, the bubbles are released to the atmosphere.

3 Next Steps

As discussed above, the present stage of model development is experimental, and future refinements to the model are anticipated. Data obtained from future field and laboratory studies will be necessary for validation of the model framework and calibration of a working model. The present study does not include model calibration or simulations, but recommendations are provided below for follow-up studies that will assist in model setup and validation. A list of potential refinements follows, based on the importance of each process and relevance to pit lake water quality.

3.1 Potential Refinements

The present model includes a framework for predictive modeling of sediment diagenesis and gas production, for oil sand pit lakes, and for other systems. In the next phase of development, the following processes could be added to the model so that it can represent these processes mechanistically:

i. Dynamic calculation of sediment pH and temperature. The diagenesis processes will affect the pH and temperature of the sediments and pore water, which may in turn affect chemical reactions through Le Chatelier's principle. This feedback loop could be included in the sediment module by calculating pH. Of particular importance is the production of CO_2 and its effect on pH and alkalinity.
ii. Metal complexation and diagenesis. Cycling of metals, such as iron and manganese, as well as the binding of these metals with sulfides and other anions could be considered in future updates.

3.2 Known Limitations

There are known limitations to the model framework where simplifying assumptions were necessary. The need for these assumptions arose because complete numerical models were not available for some processes and excessive computational effort would be required for others. These assumptions are not anticipated to prevent the model from achieving its objectives, either because they exert less influence on water quality or because they can be accounted for through calibration parameters or direct time series inputs. These are listed below so that users are aware of these limitations and can account for them in model setup or when evaluating model output. The module is limited in its ability to mechanistically simulate the following processes:

i. Consolidation of tailings.
ii. Interaction of bubbles on ice formation.
iii. Nucleation of gas bubbles.
iv. Vertical variation in sediment properties.
v. Cycling of organic compounds in sediments.
vi. Transport of bitumen and volatile organic compounds with ebullition.
vii. Consumption of oxygen due to sediment resuspension.

3.3 Validation of the Model Framework

As the first phase of development has been completed, the model can be set up and run on real-world applications. However, the first step in running the model will be to validate the model framework. The following steps are recommended to validate the model framework and ultimately set up a predictive model. Most or all of these steps will need to be completed to ensure the model is validated, defensible, and set up appropriately, prior to attempting to use it for predictive simulations:

i. Obtain reasonable estimates, where available, for all applicable inputs to the model. The primary source of this information would be tailing ponds or experimental reclamation waterbodies on existing oil sand operations, but some rates and coefficients could also be obtained from microcosm, mesocosm, and column tests.
ii. Conduct systematic sensitivity tests for a range of model variables by applying the model to a prototype, regardless of the availability of complete performance data. Results of this step would aid in the user's understanding of the model's processes and their relationships and applicable range of parameter values and would help identify process or parameterization gaps.

If any processes cannot be replicated in the model using reasonable rates and coefficients, alternate formulae may need to be incorporated into the model. After the model framework has been validated, laboratory and field studies should be conducted to derive rates and coefficients where literature values cannot be obtained or where they are found to be inadequate for the system of study. This may be done on single variables or on groups of processes, depending on the availability of data. For example, laboratory-scale tests may be used to determine the values of single variables, which can then be tested in the model.

Data that might be obtained in field studies, which were not available at the time of model development but might be significant drivers, include the following:

i. Concentrations of nutrients and carbon forms in MFT pore water;
ii. Temperature, pH, and other physiochemical characteristics of MFT pore water;
iii. Size and composition of bubbles formed by methanogenesis;
iv. Physical characteristics and variability of cracks formed by long-term bubble formation; and
v. Influence of the FFT layer on released pore water.

Other data may be more appropriately collected by laboratory studies. Such data may include the following:

i. Kinetic rates of diagenetic reactions;
ii. Inhibition (or stimulation) of methanogenesis due to the presence of nitrogen and sulfur compounds; and
iii. Enumeration of microbial functional groups, identification of key microbial genera in the sediments, and water column and their dynamics over time as the EPL matures.

4 Conclusions

The module has been developed to mechanistically model digenetic processes in oil sand pit lakes. While oil sand pit lakes and tailing ponds were the focus of the data and literature used in module development, the algorithms are generic and could be applied to other lakes with high organic matter. The module includes physico-chemical processes such as degradation of organic compounds, gas generation, bubble formation, ebullition, and gas exchange with bubbles in the water column.

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