Sediment Organic Contents Required for Gas Hydrate Formation

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Advances in basin and petroleum system modelling have allowed for the investigation of gas hydrate systems, including modelling of the generation, migration, and accumulation of biogenic and thermogenic gas within gas hydrate deposits.

methane hydrate | gas hydrate | basin modelling | organic carbon

1. Introduction

Basin and petroleum system (BPSM) modelling allows for the reconstruction of basin histories and for the reconstruction of petroleum system (including gas hydrate system) evolution [1]. In BPSM, measurements or estimations of total organic carbon (TOC) and of hydrogen (expressed as the hydrogen index, HI) are critical in assessing the generative potential of sediments or rock (i.e., how much oil and gas these sediments or rock could produce) [1]. BPSM of gas hydrates uses TOC and HI values of shallow sediments in assessing the biogenic generation of gas, and the resultant accumulation of such gas as free gas phases and/or as gas hydrate.

PetroMod™ is a comprehensive BPSM software suite that has recently been used to model the biogenic generation of gas and the formation of gas hydrate (e.g., [2][3]). The first published PetroMod™ model of gas hydrate formation modelled both shallow biogenic and deeper biogenic (as well as deep thermogenic) methane generation [2].

2. Sediment Organic Contents Required for Gas Hydrate Formation

The sediment organic contents (TOC and HI) used in previous BPSM studies are listed in **Table 1**.

Table 1. Sediment organic contents used in the modelling studies surveyed.

Reference	Location	Sediment Age	TOC (wt.%)	HI
Kroeger et al., 2015 [2]	New Zealand (Pegasus Basin)	Miocene to Recent	0.5 (conservative) 1.0	100
Fujii et al., 2016 [4]	Japan (Nankai Trough)	1.5 to 0 Ma	0.5	60

Reference	Location	Sediment Age	TOC (wt.%)	HI
Piñero et al., 2016 [3]	Theoretical layer-cake model	2.5 to 0 Ma	2.5	240
Burwicz et al., 2017 [5]	Gulf of Mexico (Green Canyon)	Pliocene and Pleistocene	0.7 (conservative) 1.0 (most realistic)	100
Crutchley et al., 2017 [6]	New Zealand (Hikurangi margin)	Miocene to Recent	0.5	100
Kroeger et al., 2017 [7]	New Zealand (Taranaki Basin)	Miocene to Recent	0.5	100
Kroeger et al., 2019 [8]	New Zealand (Pegasus Basin)	Neogene	0.5 1.0	100
Sun et al., 2020 [9]	China (Pearl River Mouth Basin)	Quaternary and older	0.5 1.0	?

The 2D BPSM model published by Kroeger et al. [2] was the first (aside from conference proceedings) to describe the use of PetroMod™'s capabilities for the modelling of gas hydrates. This model simulates both biogenic and thermogenic generation of gas, migration into the GHSZ, and formation of gas hydrates [2]. It finds that biogenic gas generation is the primary contributor to predicted gas hydrate saturations, and that this generation peaks at a depth of ~1600 mbsf [2]. Kroeger et al. [2] utilize a conservative TOC estimate of 0.5 wt.%, as well as a TOC of 1 wt.%, for biogenic gas generation in the Miocene to Recent finer-grained sediments. A standard HI of 100 was used in accordance with general marine averages for the region (Kroeger, *personal communication*). It assumed that microbial gas generation peaked at 37.5 °C (based on the 35 to 40 °C peak for microbial gas generation of [10]), and followed a Gaussian distribution [2]. Average predicted hydrate saturations are 0.9% for TOC of 0.5 wt.% and 1.6% for TOC of 1 wt.%, though it should be noted that saturations of up to 20 to 70% are predicted in accumulations influenced by structural and/or stratigraphic focusing of gas migration, and higher saturations are predicted at the base of the GHSZ [2]. It should also be noted that in the Miocene–Recent sediments, predicted masses of gas hydrate increase proportionally to the TOC contents [2]. The model was not found to reproduce any significant amount of contribution to gas hydrate formation via the shallowest gas generation (in the upper 200 m of sediment), rather, most of this gas was found to escape to the overlying water column [2].

Two models were published in early 2016, and cover 2D and 3D modelling of the Nankai Trough [4] and a theoretical 3D layer-cake model intended to demonstrate the PetroMod™ gas hydrates module [3].

The Nankai Trough IT covers the Daini-Atsumi Knoll, which includes the site of the first offshore gas hydrate production test site [4]. As per previous carbon isotope work on retrieved gas hydrate core samples, the research assumes most gas here to be biogenically sourced, and therefore models microbial generation [4]. Fujii et al. [4] use a TOC of 0.5 wt.%, based on core analysis, and use a "base case" HI of 60 for 3-D modelling. Peak microbial gas generation is modelled with a peak at 12.5 °C for the 3-D model [4]. Based on sensitivity analysis using the 2D model, use of this lower peak generation temperature is found to result in a model that much better predicts the observed accumulations of gas hydrate, whereas higher peak temperatures fail to do so [4]. In general, the model parameters utilized are found to accurately predict the locations of observed gas hydrate accumulations [4]. It notes that predicted gas hydrate saturations, some in excess of 30%, tend to correlate with sediment distribution (stratigraphic control) and formation dip direction (structural control) [4].

The theoretical model published by Piñero et al. [3] serves to demonstrate the use of the PetroMod™ gas hydrates module in simulating the distribution and temporal evolution of the GHSZ, the biogenic and thermogenic generation of gas, migration of generated gas, and the accumulation of this gas in gas hydrate deposits. It uses a TOC of 2.5 wt.% and HI of 240 (based on what the research describes as the average for phytoplankton organic matter) and Middelburg kinetics for the biogenic generation of gas within 2.5 to 0 Ma sediments [3]. The theoretical research predicts nearly equal quantities of methane to have been generated via biogenic versus thermogenic processes, with slightly more thermogenic methane generated, while the methane hydrate itself is predicted to be composed of ~55% biogenic methane and ~45% thermogenic methane [3]. Importantly, most generated biogenic gas is predicted to escape to the overlying water column, though remaining gas forms gas hydrate in situ [3]. Predicted hydrate saturations range from 0 to 50–60% and tend to be a product of layer shape (structural control) and sediment properties (stratigraphic control) [3]. Faults are demonstrated to have significant effect on saturations, with saturations adjacent faults some 20 to 30% in excess of saturations further from faults [3].

The Green Canyon 3-D BPSM research by Burwicz et al. [5] is a detailed examination of the formation and accumulation of gas hydrates observed in the area. Modelling predicts a predominance of biogenic gas hydrate, in accordance with previous work on the hydrates found here, and modelled distributions of gas hydrate match well with borehole observations [5]. The research utilizes a conservative TOC estimate of 0.7 wt.%, as well as a more realistic TOC estimate of 1 wt.%, and an HI of 100 (based on DSDP data) in modelling biogenic gas generation in Pliocene and Pleistocene sediments [5]. Piñero et al. [3] uses Middelburg kinetics to simulate the microbial generation of gas within these sediments [5]. Shallow gas found within the Pleistocene layers here is mostly sourced from in situ biogenic production, which is attributed to high sedimentation rates and high TOC contents [5]. Nearly 87% of all methane generated in the model is biogenically sourced, while some 13% is thermogenic [5]. Over 60% of total methane generated is predicted to be lost to the overlying water column, while a further 19% is lost through the sides of the model [5]. Nonetheless, appreciable quantities of gas hydrate are predicted presently, with local saturations reaching as high as 80% [5]. Highest saturations (greater than 50 to 60%) are found in depressions, i.e., topographic lows (structural control), and most gas hydrate in general is predicted to accumulate as a relatively continuous layer near the base of the GHSZ (around 500 mbsf), which is attributed to sandy sediment (stratigraphic control) at this depth, as well as methane gas recycling due to high Neogene sedimentation rates causing upward shifting of the base of the GHSZ [5]. Saturations are markedly lower, reaching a high of 5 to 8%, in the uppermost Pleistocene layers (300 to 500 mbsf) above the base of the GHSZ, which is attributed to low gas flux from underlying sediments and the drastically reduced porosities created by gas hydrate at the base of the GHSZ [5]. In general, the it notes that both the presence of gas hydrates as well as saturations on the order of 20 to 80% have been confirmed by drilling during the Join Industry Project (JIP) Leg II campaign [5].

A 2D modelling research of the Pearl River Mouth Basin was published in [9]. The research uses two TOC content scenarios, 0.5 wt.% and 1 wt.%, in simulating biogenic gas generation. It is unclear what HI is used in modelling the biogenic reaction. The scholars state that biogenic gas generation temperatures range from 35 °C to 75 °C within the study area, and therefore assume that biogenic gas generation follows a Gaussian distribution with a peak value of 55 °C. The scholars use the two TOC scenarios to compare predicted saturations with seismic inversion-based prediction of gas hydrate occurrence in the study area (as well as with core sample TOC measurements) and find that a 0.5 wt.% TOC scenario fits these observations more closely. It predicts that biogenic gas generation is distributed within the sediment from 1500 mbsf to the seafloor and that thermogenic gas generation occurs between 2300 mbsf and 6000 mbsf, and overall predicts that thermogenic gas (rather than biogenic) is the primary contributor to gas hydrate in the study area.

3. Conclusions

(A) Sediment organic contents are important: organic matter content and richness exert control on the volumes of liquid and gaseous hydrocarbons generated (which ultimately impacts gas hydrate formation).

(B) Geology is important: both stratigraphic and structural controls on gas migration and accumulation are noted within the surveyed studies. These geologic controls impact gas migration and accumulation, which ultimately influence gas hydrate formation.

(C) Basin-scale (and system-scale) investigation is important: gas does not generate, migrate, and accumulate in one dimension (i.e., in the traditional view of a single well or borehole). Gas and gas hydrate systems are dynamic, operating in three dimensions, through time.

(D) Kinetics for biogenic gas-forming reactions are poorly defined and often left open to interpretation at the discretion of scholars within the surveyed studies. Improved biogenic gas kinetics are necessary to better understand and predict gas hydrate formation.

(E) Calibration matters: testing multiple scenarios for organic contents in a study area (as well as multiple scenarios for any parameter in the broader basin and hydrocarbon system, e.g., heat flow, lithology, sediment–water interface temperature, rock properties) can yield a better fit between model predictions and observations.

(F) The distribution of studies harnessing basin and hydrocarbon system modelling of gas hydrate systems is limited, and overall, relatively few studies have used basin and petroleum systems modelling-based approaches to investigate gas hydrate systems. This invites much-expanded investigation of gas hydrate systems in additional locations and additional geological contexts.

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