Marine and Petroleum Geology 71 (2016) 288–295

Contents lists available at ScienceDirect

Marine and Petroleum Geology

journal homepage: www.elsevier.com/locate/marpetgeo

Research paper

3-D numerical modelling of methane hydrate accumulations using PetroMod

Elena Piñero [a, *], Christian Hensen [a], Matthias Haeckel [a], Wolf Rottke [b], Thomas Fuchs [b], Klaus Wallmann [a]

[a] GEOMAR Helmholtz-Zentrum für Ozeanforschung Kiel, Wischhofstr. 1-3, 24148, Kiel, Germany
[b] Schlumberger GmbH, Zweigniederlassung Aachen, Ritterstr. 23, 52072, Aachen, Germany

ARTICLE INFO

Article history:
Received 7 May 2015
Received in revised form
8 December 2015
Accepted 24 December 2015
Available online 29 December 2015

Keywords:
Gas hydrates
PetroMod®
3D petroleum system modelling
Biogenic methane
Thermogenic methane
Kinetics
Migration
Fault

ABSTRACT

Within the German gas hydrate initiative SUGAR, a new 2-D/3-D module simulating the biogenic generation of methane from organic matter and the formation of gas hydrates has been developed and included in the petroleum systems modelling software package PetroMod®. Typically, PetroMod® simulates the thermogenic generation of multiple hydrocarbon components (oil and gas), their migration through geological strata, finally predicting oil and gas accumulations in suitable reservoir formations. We have extended PetroMod® to simulate gas hydrate accumulations in marine and permafrost environments by the implementation of algorithms describing (1) the physical, thermodynamic, and kinetic properties of gas hydrates; and (2) a kinetic continuum model for the microbially mediated, low temperature degradation of particulate organic carbon in sediments. Additionally, the temporal and spatial resolutions of PetroMod® were increased in order to simulate processes on time scales of hundreds of years and within decimetres of spatial extension. In order to validate the abilities of the new hydrate module, we present here results of a theoretical layer-cake model. The simulation runs predict the spatial distribution and evolution in time of the gas hydrate stability field, the generation and migration of thermogenic and biogenic methane gas, and its accumulation as gas hydrates.

1. Introduction

Gas hydrates are ice-like compounds formed by methane and water. They are stable under conditions of low temperature and high pressure, which are the main control parameters for their formation besides the presence of sufficient amounts of methane (e.g. Tishchenko et al., 2005; Marquardt et al., 2010).

During the last decades, the scientific community dedicated a strong effort to quantify the global methane resources bounded as gas hydrates in marine sediments (e.g. Milkov, 2004; Dickens, 2011; Wallmann et al., 2012). Although a consensus value around 10,000 Gt of C stored in gas hydrates was acquired ten years ago, recent estimations of the global budget of gas hydrates seems to be further below this value, predicting around 1–3 thousands of Gt of C (e.g. Burwicz et al., 2011; Wallmann et al., 2012; Piñero et al., 2013). Most of the previous estimates of gas hydrate budgets were based on the extrapolation of measured concentrations in enriched areas, which lead to excessive assessments. Later quantifications were done under 1-D transport-reaction models, with more accurate results. Only in the last few years there have been developed 2-D models dealing with gas hydrate accumulations in continental margins. However, these results have not been extrapolated to global quantifications due to the lack in the global distribution of important parameters and contour properties (e.g. Schnürle and Liu, 2011; Archer et al., 2012; Chatterjee et al., 2014). Several 1-D to 3-D models simulating methane production from gas hydrates have been published, although most of them impose a fixed geological structure over the modelled time, and/or assume a fixed initial concentration of methane hydrate or gas without modelling sediment deposition, organic matter degradation nor methane gas generation (e.g. Myshakin et al., 2012; Reagan et al., 2015).

Abbreviations: GHSZ, Gas Hydrate Stability Zone; T, Temperature; P, Pressure; TOC, total organic Carbon; PVT, Pressure/Volume/Temperature; HI, Hydrogen Index; HC, Hydrocarbons; mbsl, metres below sea level; Gt of C, Gigatones of Carbon.

* Corresponding author.
E-mail addresses: epinero@geomar.de (E. Piñero), chensen@geomar.de (C. Hensen), mhaeckel@geomar.de (M. Haeckel), wrottke@slb.com (W. Rottke), tfuchs@slb.com (T. Fuchs), kwallmann@geomar.de (K. Wallmann).

http://dx.doi.org/10.1016/j.marpetgeo.2015.12.019
0264-8172/

Even though the extrapolation of 1-D model results and similar methods may be an efficient solution to predict the gas hydrate distribution on the global scale, these may not be the best approach for regional quantifications. Gas hydrates are typically not homogeneously distributed in marine sediments because lateral variations of the control parameters such as T, P, TOC, reservoir rock distribution, etc. Hence, regional basin models are clearly advantageous for the simulation of gas hydrate accumulations, because they account for variations in the geological framework, as well as lateral variations over time of the control parameters. In such settings, the presence of faults and other preferential migration pathways can produce a big effect on gas hydrate distribution (e.g. Daigle and Dugan, 2010).

In order to tackle this challenge, a new Gas Hydrate module has been included in PetroMod®, a multidimensional petroleum system modelling package typically simulating the formation, migration and accumulation of hydrocarbons (oil and gas, e.g. Hantschel and Kauerauf, 2009). In order to discuss the capabilities of this new software tool, we present here results of the simulation of a theoretical simple 3-D model including: thermogenic and biogenic methane formation, migration pathways, evolution over time of the GHSZ, as well as gas hydrate saturation, and the total mass of methane in gas hydrate. The effect of gas migration through faults in the accumulation of methane hydrates is further discussed.

2. New developments in PetroMod®

The PetroMod® software package fully integrates seismic, stratigraphic and geological interpretations into multi-dimensional simulations of thermal, fluid-flow and petroleum migration history in sedimentary basins. PetroMod® is primarily used in hydrocarbon exploration, but has also proven to be a valuable tool in research applications (e.g. Grassmann et al., 2010; Schenk et al., 2012; He et al., 2014).

PetroMod® can be applied in new exploration areas, where only few data are available, as well as in already explored areas. Provided that the data base is sufficient, problems such as source-reservoir correlations, seal efficiencies, and overpressure systems can be investigated in order to obtain the most accurate prediction of timing and location of petroleum generation, expulsion and migration processes (e.g. Piñero et al., 2014; Kroeger et al., 2015). PetroMod® includes several migration methods to simulate fluid flow: Flowpath (buoyancy driven), Darcy flow (fluid pressure potential driven), invasion-percolation (capillary pressure driven), and a hybrid Darcy/Flowpath (Hantschel and Kauerauf, 2009). The whole petroleum migration modelling is fully PVT -controlled with multi-component relationships using flash calculations. The equation of state for methane assumed per default in PetroMod is Peng-Robinson. The results of the simulations are visualized with several overlays like the Petroleum saturation and the in-situ masses of each component.

For each time step, PetroMod first simulates the new position of each cell, performing the correspondent deposition or erosion occurring during this time step. Then the pressure of each cell is calculated (by solving the differential pressure equation) taking into account the corresponding properties of the assigned lithology (permeability, compressibility, density, etc.) and the pressures of the previous time step. Next, the porosities are updated and compaction is performed. Afterwards, temperatures are calculated (by solving the differential heat equation) taking into account the thermal properties (thermal conductivity, heat flux, heat capacity, etc.) and the temperatures of the previous time step. Subsequently, hydrocarbons generate in each cell depending on T and P conditions. Secondary cracking and adsorption are applied to the generated hydrocarbons and the not adsorbed amounts are expelled into the free pore space and migrate due to the chosen migration method, generating a fluid flow. Finally, gas hydrates will form if the cell position is inside the GHSZ and if the methane concentration exceeds methane solubility. For further information about PetroMod, the reader is referred to Hantschel and Kauerauf, 2009.

2.1. Geological model

The simple model shown below represents an area of 10 km per 5 km (Fig. 1), including fifteen layers. With a constant water depth of 800 m, it simulates the deposition of 1160 m of sediments over time. Lateral resolution is 100 m × 100 m, while vertical resolution is defined by the thickness of each layer (Table 1). The thickness of the layers increases with depth from 20 m at the shallow layers, up to 140 m at the basement layer. The lithology of the layers are defined as default lithologies and parameters included in PetroMod®. All layers in the model are siltyclay except for Layer 6, which is composed of sandstone and acts as reservoir. The homogeneous TOC content of the five uppermost layers is 2.5%, with a HI of 240 mg HC/g TOC, corresponding to the generation of hydrocarbons after the decomposition of averaged phytoplankton organic matter (e.g. Schulz and Zabel, 2006):

$$C_{106}H_{263}O_{110}N_{16}P \rightarrow 53CO_2 + 53CH_4 + 16NH_3 + H_3PO_4$$

Layers 11 and 12 act as petroleum source rocks for thermal generation of gas with a TOC content of 5.5% and HI of 480 mg HC/g TOC, a relatively low value for marine Type II formations (e.g. Hartman-Stroup, 1987). Middelburg kinetics for the degradation of organic matter at low temperature (Section 3) is applied to Layers 1 to 5. A standard thermogenic kinetic rate law (modified from Krooss et al., 1993) is applied to the source rock (Layer 11 and 12, Table 1), with activation energies ranging between 39 and 67 kcal/mol and a frequency factor of 2.28×10^{25} $Myrs^{-1}$ (Table 2).

The depositional intervals of the layers increase gradually with depth up to 10 Myrs (Table 1), generating an averaged sedimentation rate of ~5 cm/kyr, with values ranging from 1.4 cm/kyr in the basement to 10.4 cm/kyr in layer 4, right above the anticline. The heat flow is homogeneous (50 mW/m^2) and constant for the whole modelled time. The temperature at the seafloor gradually decreases from 15 °C (55 Myrs ago) to 4 °C, which is constant for the last 15 Myrs (Fig. 2).

In order to study the effect of preferential fluid migration through geological conduits, two vertical faults of ~3 km length were implemented in the model (Fig. 1). In our simple model, faults are treated as Boundary Elements; it is high permeability surfaces, without volume, and without considering rock or sediment displacement. Fault 1 has a NNE-SSW direction in the eastern half of the modelled block. It cuts Layers 4 to 10, from 860 mbsl down to 1275 mbsl. Fault 2 has a NW–SE direction, on the western part of the block. It breaks through layers 3 to 13, from 840 mbsl and down to 1600 mbsl. PetroMod® includes several ways to define fault properties. In this particular model, fault capillary pressure (Hg-air) for both faults was homogenously set to 7 MPa, which corresponds to a medium value in the range normally used in petroleum systems modelling (0.01–100 MPa), corresponding to the lower range of open faults (e.g. Hantschel and Kauerauf, 2009).

3. New 'gas hydrate' module

To develop the new gas hydrate tool in PetroMod® the software has been extended with: i) routines for the physical and thermodynamic properties of methane hydrates; ii) kinetic formulation for the formation and dissociation of gas hydrates through time; iii)