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## Flow simulation with reactive transport applied to carbonate rock diagenesis

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#### **ABSTRACT**

Significant volumes of the known hydrocarbon reserves are found in carbonate rocks, many of these dolomitized. The spatial distribution of diagenesis on these rocks is one of the main challenges in oil reservoir modeling. Reactive transport models can be a powerful tool to understand the active diagenetic processes and their effects on the quality of these reservoirs. In this study it was used, for the first time, the CMG-GEM simulator to model diagenetic evolution of a carbonate sequence, subjected to compaction-driven and geothermal flow in a simulated period of 200 thousand years. It was simulated carbonate cementation, dolomitization and dissolution, with and without presence of faults. Among the analyzed variables, the volume of circulating fluid was the most important factor. For both mechanisms, flow simulated velocities obtained had magnitudes smaller than  $10^{-6}$  m/day. Diagenesis was insignificant for these low speeds at simulated time interval. Only dolomitized facies presented relevant diagenesis in form of calcite dissolution and dolomite precipitation. Simulations with flow rates of 1 m/ day revealed a considerable increase in observed diagenesis, especially in carbonate cementation and in porosity enhancement. Diagenesis was more pronounced in more permeable sediments, highlighting the role of fluid flow in diagenetic reactions. Relative dissolution was greatly reduced during simulations performed with absence of dolomite and dolomitization reactions. The presence of faults strongly influences spatial distribution of diagenesis, especially relatively to dissolution. More permeable facies were more dissolved near fault, decreasing with increasing distance. Low permeability facies, as mudstones, are not dissolved, even near fault. Spatial distribution of diagenesis would then be dependent mainly on the quality of original pore structure, of fault presence and mineral composition of rock.

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#### 1. Introduction

Diagenetic processes in sedimentary basins involve reactions between pore water and rocks mineral phases, while unstable minerals are dissolved more stable phases precipitate. As these reactions have thermodynamic and kinetic control, the processes can be reproduced with the application of numerical models ([Bjorlykke et al., 1988; Ronchi et al., 2012\)](#page--1-0). A growing number of works have been published in recent years providing several conceptual models for diagenesis in carbonates, ranging from simple mass balance calculations ([Whitaker et al., 1999](#page--1-0)) or simple flow models with restricted boundary constrains [\(Jones et al., 2000\)](#page--1-0) to more complex models with reactive transport equations [\(Whitaker](#page--1-0)

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#### [et al., 2004; Whitaker and Xiao, 2010; Ronchi et al., 2012; Xiao et al.,](#page--1-0) [2013\)](#page--1-0).

Reactive transport modeling (RTM) is a set of interpretive tools to unraveling the complexities of carbonates diagenesis coupled processes, in order to deduce their effects in space and time in a variety of scales ([Bethke, 1996; Steefel et al., 2005\)](#page--1-0). Two different mathematical approaches are merged in reactive transport modeling. The first one is the physical modeling of mass and heat transport, which aims to represent the material and energy flow in a variety of geological scenarios. In physical modeling, the aim is to simulate different flow patterns acting in the sedimentary basin and quantify limitations applicable to these patterns in terms of flow velocity and total volume [\(Bjorlykke et al., 1988\)](#page--1-0). These flow patterns will be directly related to diagenetic environments and some of which can be seen on different environments. Three main patterns of water flow can be identified in sedimentary basins and will act in diagenesis [\(Bjorlykke et al., 1988; Whitaker et al., 2004](#page--1-0)): \* Corresponding author.



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Flow driven by differences in densities of pore fluids due to differences in temperature or salinity/ion concentration; Pore-water flow driven by rock compaction and porosity loss in sediments with increasing burial; Flow driven by differences on hydrostatic head defined by the elevation of the ground water table above sea level. The other approach is the geochemical modelling, used to capture key characteristics of diagenetic processes, such as chemical leaching, hydrothermal alteration and dolomitization, among others ([Ronchi et al., 2012; Xiao et al., 2013](#page--1-0)). In other words, geochemical modelling tries to represent mathematically the rockfluid interaction ([Steefel et al., 2005; Al-Helal et al., 2012](#page--1-0)).

Flow simulation combined with rock-water interaction reactions in RTMs can be a useful method to decide between several hypotheses of diagenetic settings, which are more compatible with field data and to select which is the best model that fits mass balance, chemical kinetics and thermodynamic constraints ([Bethke,](#page--1-0) [1996; Whitaker et al., 2004](#page--1-0)). The simulator CMG-GEM applies finite difference method to perform flow simulations in porous media, heat flow, equilibrium reactions and kinetics with mineral precipitation and dissolution [\(Nghiem et al., 2011](#page--1-0)). Although several studies have used CMG-GEM to simulate rock-fluid interaction during hydrocarbon production ([Alexander and Boodlal,](#page--1-0) [2014; Qiao et al., 2014](#page--1-0)) and  $CO<sub>2</sub>$  storage in sedimentary rock ([Nicot et al., 2009\)](#page--1-0), there are no references of its use in diagenetic simulation.

This study presents the results of several simulations of an Albian carbonate reservoir diagenetic evolution using the commercial compositional simulator CMG-GEM combined with a petrological study. The main goal was to evaluate if the tools provided by CMG-GEM can simulate most of the physical phenomena and chemical reactions applied to diagenetic processes, especially the ones related with cementation and dissolution.

#### 2. Methods

#### 2.1. Geological settings

Campos Basin is a sedimentary passive margin basin, and its formation started from the event rift that splits Gondwana supercontinent giving rise to African and South American continents ([Spadini et al., 1988; Dias et al., 1990; Milani et al., 2000; Winter](#page--1-0) [et al., 2007\)](#page--1-0). Immediately after deposition of the post-rift supersequence, characterized by an evaporitic event in the transition from Aptian to Albian ages, it was formed a narrow inland sea characterized by a thick layer of carbonate sediments that extends to the end of the Albian age ([Ojeda, 1982; Dias et al., 1990; Spadini](#page--1-0) [et al., 1988\)](#page--1-0), corresponding to Macae Group, which comprises the Quissamã Formation, object of this study.

The lower portion of Quissama formation has as lower limit the evaporitic event in the transition from Aptian to Albian and is characterized by a tidal flat carbonate system ([Spadini et al., 1988;](#page--1-0) [Mohriak et al., 1990; Winter et al., 2007](#page--1-0)). In the intermediate portions of the sequence, carbonate sediments deposited from average to high energy environment, represented by oolitic shoals, oncolytic and peloids with varied porosities are prevailing ([Winter et al.,](#page--1-0) [2007; Okubo et al., 2015](#page--1-0)). The high energy facies were deposited on the structural highs, characterized as shoals, in which higher energy facies, as the ooids, occupy the shoal center, while oncolytic facies was deposited on the flanks, under moderate energy conditions ([Robaina et al., 1991\)](#page--1-0).

[Okubo et al. \(2015\)](#page--1-0) highlighted as the main diagenetic processes recognizable in carbonates from Quissama formation: micritization, recrystallization, calcite cementation, dissolution, dolomitization and compaction. According to [Winter et al. \(2007\),](#page--1-0) the oolitic/oncolytic banks shows variable porosity, and the porosity observed is generally interparticle, intercrystalline, vuggy or moldic, the first predominating ([Okubo et al., 2015\)](#page--1-0). Cycles of upward shallowing have more fine-grained sediments at the base and clean sediments at the top of the cycle: peloidal packstones on the basis of cycles have porosities of 30%, while the oolites grainstones from the top shows even higher porosities ([Okubo et al., 2015](#page--1-0)). Intense dolomitization is observed on the formation basis near salt layer, being attributed to its origin evaporitic environmental conditions at the time of deposition ([Spadini et al., 1988; Okubo et al., 2015\)](#page--1-0). Subsurface diaganesis appear mainly in form of compaction and carbonate cementation of grainstones [\(Okubo et al., 2015](#page--1-0)).

#### 2.2. Petrography

Thin sections were prepared from 148 samples of rock from three wells P1, P2 and P3 drilled into an oil reservoir belonging to Quissamã formation. The thin sections were stained with alizarin to facilitate differentiation between calcite and dolomite. A general picture of each slide was obtained, with an enlargement of 21,25X and 4 detail pictures, with an enlargement of 85X. Each thin section analyzed was photographed with a resolution of 0.008 mm/pixel photomicrographs for 21,25X enlargement and 0.002 mm/pixel for 85X enlargement. For more heterogeneous slides were obtained up to 8 detail photos. With the aid of ImageJ image processor ([Igathinathane et al., 2008](#page--1-0)) were selected and quantified in the photographs the characteristics of the rock features that were wanted to quantify: total porosity and intergranular porosity, calcite cementation and dolomite cementation.

#### 2.3. Simulation

The software used was CMG-GEM that uses finite difference method to perform flow simulation, heat flow, equilibrium and kinetics reactions with mineral precipitation and dissolution ([Nghiem et al., 2011\)](#page--1-0). Simulations were performed considering the flow mechanisms by geothermal convection and compactiondriven flow, separately and combined. Other variables tested were: initial porosity and permeability, reactive surface, presence of dissolved  $CO<sub>2</sub>$  in water and dolomite reaction. The simulation was performed by the following steps:

#### 2.3.1. Model grid

The simulation model consists of 24300 cells, each one with  $10 \times 10 \times 1$ m dimensions, arranged to represent a schematic section of the studied area [\(Fig. 4\)](#page--1-0); well P1 was used as a stratigraphic reference. The evaporite layer underneath carbonates sediments was considered as the model lower boundary. Three main grainstone banks were identified in well logs and thin sections and were represented in the section [\(Fig. 1](#page--1-0)). Lower grainstone bank was differently represented in the model due to its high dolomitization average (20%). Incipient dolomitization was found on the upper banks, but was not considered in simulations ([Fig. 1](#page--1-0)).

The reservoir burial depth average is 4,000 m. The preliminary quantitative diagenetic studies from thin sections indicate that pore structure was preserved by cementation in grainstones and packstones at burial depths between 1500 and 2,600 m. Therefore, simulations were performed considering a burial depth average of 2,000 m. Due to limitations imposed by computational performance, simulated time interval was 200,000 years.

#### 2.3.2. Porosity and permeability

Porosity was calculated as a function of depth using the relationship shown in equation (1):

$$
\Phi = \text{PO} \exp(-bZ) + \text{P1} \tag{1}
$$

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