Compositional Simulation of Petroleum Vertical Migration and Evaporative Fractionation Processes*

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Abstract

Petroleum systems modeling allows the dynamic simulation of a series of physical and chemical processes during the geological history of a sedimentary basin. Among these processes, physical and chemical changes in petroleum associated with vertical migration are of utmost importance for the assessment of petroleum volumes and composition in an exploratory context. Evaporative fractionation is one of the processes related to petroleum migration, which may cause alterations in the composition of an accumulation. Evaporative fractionation can be characterized by a quantitative analysis of chromatographic and PVT fluid data. This phenomenon can be simulated by coupling equations of multicomponent flow with equations of state in a petroleum systems simulator.

Several studies have confirmed, by the analyses of reservoirs fluid data and laboratory scale experiments, the occurrence of evaporative fractionation in basins. In order to verify whether a basin simulator is able to replicate the effects of evaporative fractionation during petroleum vertical migration, tests were performed using a synthetic geological model built in the PetroMod v.2011 software (IES/Schlumberger). A hybrid method of migration was used that combines multiphase Darcy flow (for lithologies with permeabilities less than 100 mD) and ray tracing (for carrier rocks), with petroleum composition based on a kinetic scheme with eleven compound classes, which is representative of the PVT properties of lacustrine oils from Brazilian marginal basins. PVT calculations (phase separation, physical and chemical properties of each phase) must be undertaken for each accumulation during the whole model history.

Evaporative Fractionation

Thompson (1987 and 2010) defined evaporative fractionation as a product of either gas injection (forced depletion), or reservoir decompression (self-depletion), in an oil accumulation, followed by phase destabilization/separation and gas escape, which carries upwards the light fractions derived from the oil in solution. Together with the loss of light fractions in the residual oil, there is an increase in the content of light aromatic and naphthenic compounds relative to linear paraffins in the residual oil and successively derived gas condensates, which allows the distinction of evaporative gas condensates from those generated by thermal cracking (Thompson, 1987).

Synthetic Geological Model

To build the synthetic geological model, as well as for the flow simulation and numerical tests, the PetroMod (v.2011) software was used. The synthetic model has an area of 32 x 32 km and maximum depth of 7 km, discretized into a numerical array of 23,808 cells. The model is primarily characterized by stacked pairs of a sandstone layer with petrophysical properties of a reservoir rock overlain by a shale layer with properties that mimic the behavior of a seal rock. For the basal layer of the model, a shale source rock was defined. The various layers comprise a domic structure with its apex at the center of the model that was developed during a total model history of 125 Ma (Figure 1).

As boundary conditions for the thermal calculations, constant values for sea-bottom temperatures (4°C) and basal heat flow (80 mW/m^2) were used. For the source rock layer, values of 20% total organic carbon and a hydrogen index of 400.4 mg HC/gTOC were used.

Simulated Scenarios

Six scenarios were performed to test variations in the capillary pressure of the deepest seal layer and in the kinetics of petroleum generation and cracking. In scenarios 1, 3 and 5, a capillary pressure similar to that of salt was assigned to the deepest seal layer, resulting in a single petroleum accumulation in the deepest reservoir layer of the model. In scenarios 2, 4 and 6, all the seal layers behave similarly, with capillary pressures equivalent to those of shale, thus allowing the simulation of a stack of petroleum accumulations. Modeling results of the successive formation of petroleum accumulations, their volumes, filling and leakage histories, as well as the changes in petroleum fluids (phases, physical properties and their chemical compositions), have been analyzed through time and space in all tested scenarios.

Regarding the kinetics of primary cracking in the source rock, the compositional scheme from Penteado and Araujo (2009) was used, which was developed to account for the composition of petroleum generated by lacustrine source rocks in the marginal basins in southeastern Brazil. This scheme is characterized by ten classes of compounds for primary cracking, including the gaseous (C_1, C_2 and C_3-C_5) and liquid (C_6-C_{60}^+) fractions. The compositional scheme also includes the kinetics of late C_1 generation from refractory kerogen, in addition to the parameters for secondary cracking of the C_2 to C_{60}^+ compound classes.

Scenarios 1 and 2 were simulated using only the compositional kinetics for primary cracking. For scenarios 3 and 4, the kinetic scheme for primary cracking was coupled with late methane generation. Finally, scenarios 5 and 6 were simulated through the use of the full kinetic scheme, including primary cracking, late methane generation and secondary cracking of compound classes both within and outside the source rock.

Results and Conclusions

In scenario 1 (Figure 2), the single oil accumulation in the deepest reservoir remains monophasic with a constant composition (26.8° API gravity and gas-oil ratio – GOR – of 100.6 m^3/m^3) throughout the model history because the mass fractions of the compound classes are the same for all activation energies in the kinetics for primary cracking.

Scenario 2 also considers the kinetics for primary cracking only, but in this case, the lower capillary pressures in the seals favor petroleum vertical migration (Figure 2). The deepest accumulation in this scenario closely resembles its counterpart in scenario 1. Four other accumulations are formed above, with slightly greater API gravities and lower gas-oil ratios (between 35 and 100 m^3/m^3). These upper four accumulations are a result of the breach of the capillary barrier of the first seal layer. As a consequence, vertical migration of oil from the deepest accumulation occurs, producing the accumulations above. As petroleum moves upwards, phase separation takes place in some of these shallower reservoirs, and the gas-condensate (API = 56º and gas-oil ratio > 24,000 m^3/m^3) cap is partly lost to higher reservoirs and to the surface. Later, progressive burial, with its accompanying increase in seal capillary pressure, prevents further losses. The modeled composition of the petroleum lost in the top of the model (more than 87% C_1-C_5 gaseous compounds) corroborates the interpretation that it was derived from underlying gas caps. The model thus was able to simulate the occurrence of evaporative fractionation by decompression, phase separation and loss of the lighter fractions through the disrupted seal layer (self-depletion).

Scenario 3 (Figure 2) differs from scenario 1 by the inclusion of late methane generation. The single accumulation formed in scenario 3 is like its equivalent in scenario 1 until the onset of late methane generation, which causes an increase in gas-oil ratios until a phase separation occurs. Subsequent burial induces progressive changes in composition and physical properties of the gas and liquid phases.

The main difference between scenarios 2 and 4 is the addition of late gas generation in the latter. Initially, accumulations are formed above the deepest reservoir by decompression and phase separation, with leakage of the gas cap through the seal. However, the additional late methane causes more dry gas to move upwards, leading to phase separation in almost all the accumulations, gas washing of the lighter oil fraction and enhanced vertical migration, with seven accumulations formed (Figure 2). The injection of more methane in the system increased the overall API gravity (between 27º and 55º) and gas-oil ratios (between 130 and 2,900 m^3/m^3) of the upper accumulations. This suggests that late methane is responsible for carrying the lighter fractions of petroleum towards the top. Therefore, the results of scenario 4 demonstrate that the process of evaporative fractionation by forced depletion can be adequately modeled.

Among all the scenarios resulting in a sole petroleum accumulation (1, 3 and 5), scenario 5 is the only one that takes into account the secondary cracking of C_2^+ compounds. In scenario 5, the evolution of the petroleum phases and compositions parallels those of scenario 3 until secondary oil cracking starts under reservoir temperatures greater than 170°C. Thereafter, GOR and API gravities increase in the liquid phase until it is completely cracked. Ultimately, the accumulation is composed uniquely of methane.

Finally, in scenario 6, the phases and compositions in all the accumulations are a result of a complex interaction of evolving fluids with vertical migration processes. Most of the above-mentioned phenomena occur partially overlapping in time. The result of the scenario 6 is a stratified pattern of accumulations: the lowermost reservoirs contain essentially gas; intermediary reservoirs are filled by volatile oils; and the shallower reservoirs contain only gas condensates.

The results of the six modeled scenarios have shown that during the supply dynamics of increasingly evolved petroleum charges to several stacked traps, petroleum vertical migration is a highly complex process as a function of: 1) capillary seal breach induced by underlying petroleum accumulations; 2) phase separations during vertical migration; 3) leakage of gas caps through seals and losses to the surface; 4) gas washing caused by upward migration of late methane sweeping light compounds upwards, and 5) progressive cracking of heavier compound classes as accumulations are buried deeper. Our models were able to simulate the occurrence of evaporative fractionation both by decompression (phase separation or self-depletion) and by gas washing (forced depletion). Thus, the numerical experiments performed here have shown that evaporative fractionation can be adequately reproduced in the scale of petroleum systems modeling, and be used to assess its effects on fluid composition in exploration prospects.

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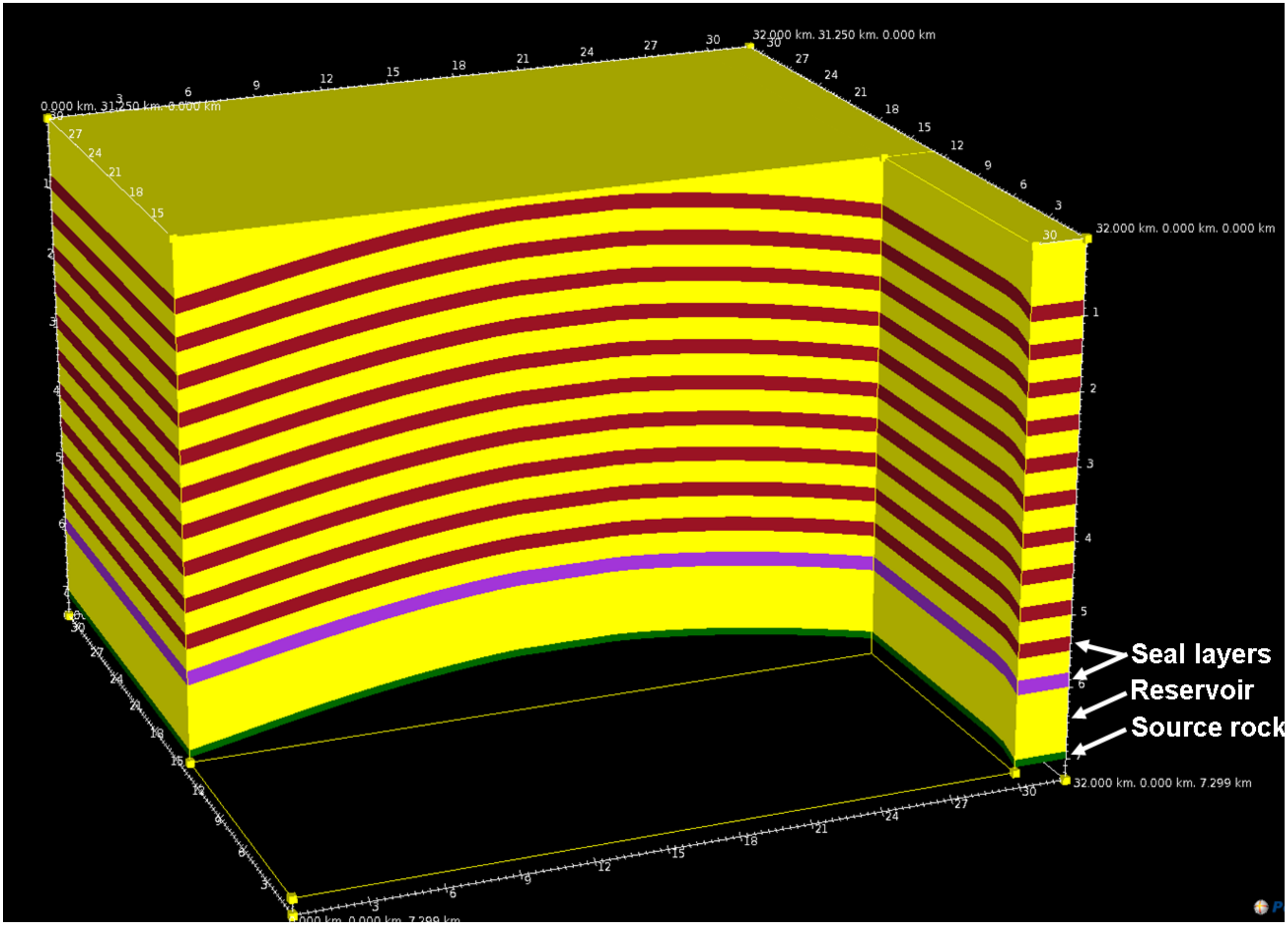

Figure 1. Synthetic geological model showing the stack of reservoir (sandstone) and seal (shale) layers. At the base of the model, the source rock layer.

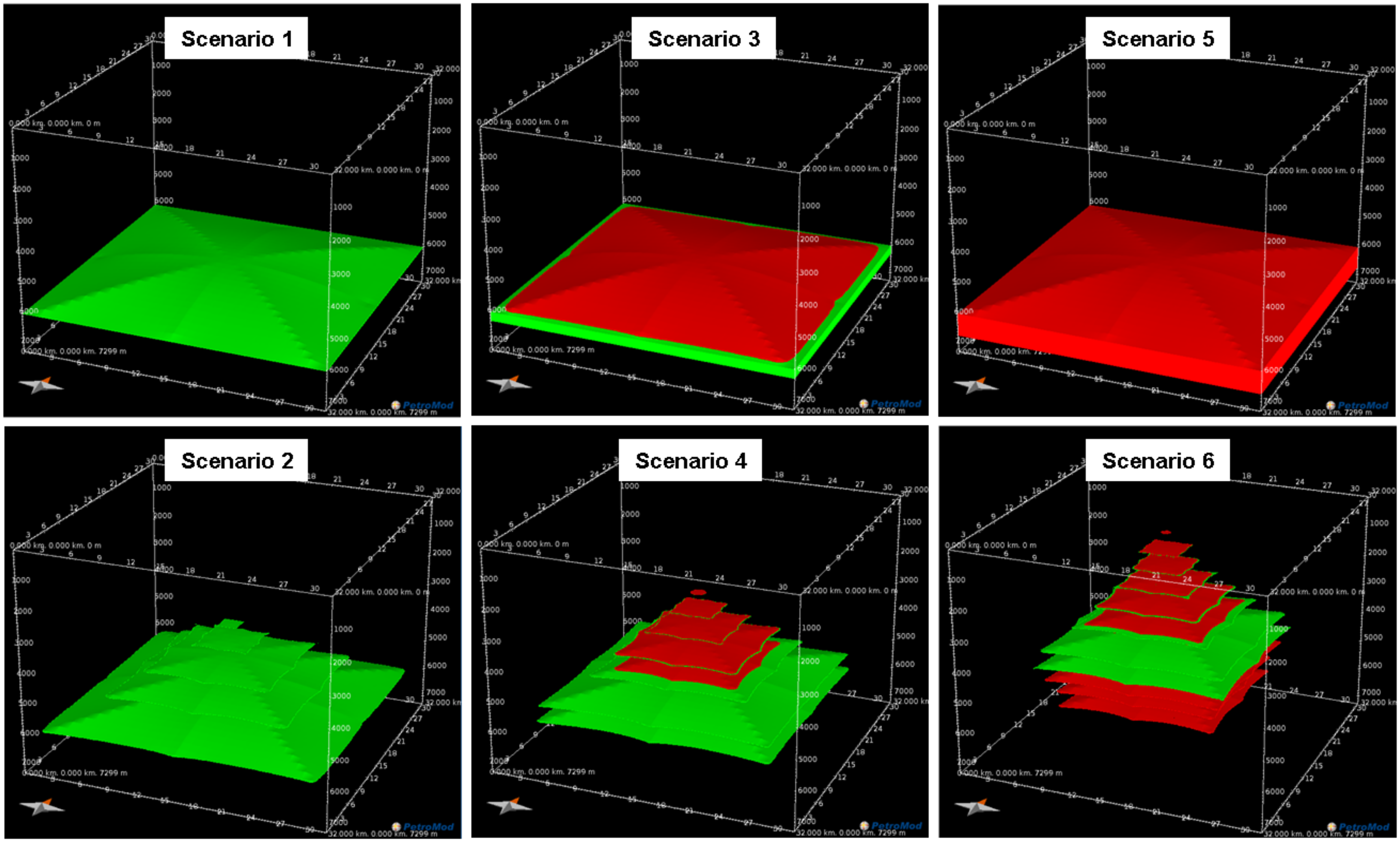

Figure 2. Petroleum accumulations resulting from the different modeling conditions of scenarios 1 to 6. Liquid accumulations shown in green, and gas in red.