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PIT (Petroleum Inclusion Thermodynamic): a new modeling tool for the characterization of hydrocarbon fluid inclusions from volumetric and microthermometric measurements

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Abstract

A recent technique, the confocal scanning laser microscopy, allows for the accurate measuring of the bubble filling degree (F_v) of oil fluid inclusions as a function of the temperature [Pironon, J., Canals, M., Dubessy, J., Walgenwitz, F., Laplace-Builhe, C., 1998. Volumetric reconstruction of individual fluid inclusions by confocal scanning laser microscopy. Eur. J. Mineral. 10, 1143–1150]. These data, combined with measurements of homogenization temperature (T_h), give us new constraints for characterizing individually hydrocarbon fluid inclusions. For this purpose, a new modeling tool, PIT (Petroleum Inclusion Thermodynamic), based on applied thermodynamics of natural oils, has been constructed for interpreting volumetric (F_v) and microthermometric (T_h) measurements obtained on hydrocarbon fluid inclusions. The software allows us: (1) to reconstruct the paleo-thermobarometric trapping conditions of oils; (2) to model petroleum inclusion composition; and (3) to understand (F_v–T_h) differences among a population of fluid inclusions in terms of various pre- or post-trapping processes (inclusion stretching, oil mixing, liquid/vapor de-mixing, oil leaching by a gas, etc.).

Keywords: hydrocarbons; fluid inclusions; microthermometry; oil migration; modeling; fluids; equations of state

1. Introduction

Hydrocarbon fluid inclusions are valuable objects to provide important information about pressure–temperature conditions of oil migration in sedimentary basins because aliquots of oils that have migrated are often trapped in fluid inclusions. However, oil fluid inclusions are not easy to characterize, mainly because of their compositional complexity. Recently, analytical techniques (FT-IR, Raman, UV fluorescence) have been applied to oil fluid inclusions. However, it is still difficult to interpret these measurements in terms of useful geochemical parameters for every case of fluid inclusion study.

A new technique, the "confocal scanning laser microscopy coupled with hydrocarbon fluorescence" (Pironon et al., 1998), has made it possible to measure accurately the gaseous filling degree (F_v) of oil fluid inclusions (Fig. 1) at any temperature (below the homogenization temperature, T_h). Combined use of this technique with conventional microthermometry,

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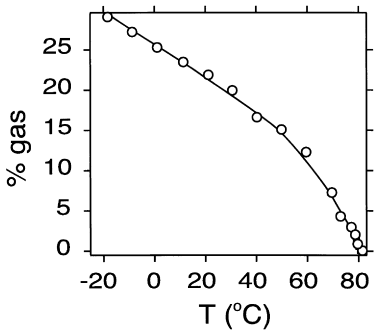

Fig. 1. The variation of the gaseous filling degree (F_v) as a function of the temperature. Empty circles are data measured by confocal scanning laser microscopy on an oil fluid inclusion, homogenizing at 81.6°C.

could give us indications about the compositions (x) and P–T trapping conditions (P_t–T_t) of oil fluid inclusions (Fig. 2).

The $F_v(T)$ curve depends both on the density and composition of trapped oils. Thus, these volumetric data, combined with homogenization temperatures (T_h), provide us new constraints for determining the composition of fluids and reconstructing the isochoric paths of fluid inclusions. A first software, VTFLINC (Aplin et al., 1999), has already been developed for this purpose. We propose here a new modeling tool,

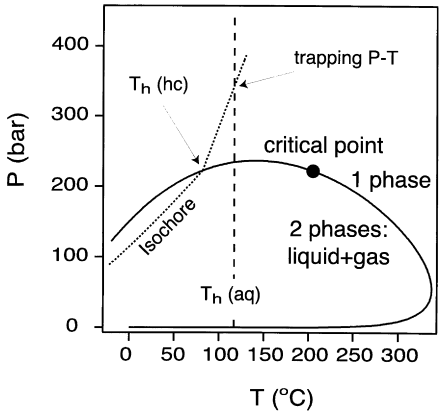

Fig. 2. The P–T phase diagram of an oil fluid inclusion, showing its homogenization point (T_h), its isochoric path, and its trapping point (P_t–T_t). The homogenization temperatures of associated aqueous fluid inclusions (which are assumed to be contemporaneous with oil fluid inclusions and methane saturated) usually give trapping temperatures. Trapping pressures are simply read along the isochoric path.

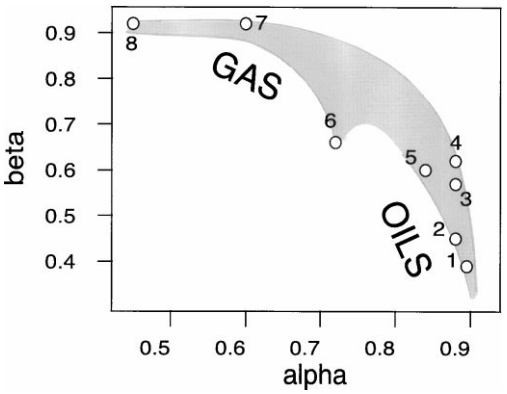

Fig. 3. The α–β diagram showing the general correlation existing for a wide range of natural hydrocarbons: (1) heavy oil; (2) CO_2-rich oil; (3) light oil; (4) light oil; (5) "critical" oil; (6) gas condensate; (7) wet gas; and (8) dry gas. Lines drawn are general trends (explained in the text).

called PIT (Petroleum Inclusion Thermodynamic), with improved capabilities for the study of petroleum fluid inclusions.

2. Composition modeling of oils

Oils are complex fluids, which contain thousands of components (paraffins, naphtenes, aromatics, etc.). Conventional chemical analyses are not sufficient to characterize such mixtures, and new compositional parameters must be defined to describe a natural oil in its main lines. For this purpose, experience gained in the oil industry is extremely valuable, and a compositional model (Montel, 1993), used intensively for the characterization of petroleums, has been applied. This model is able to represent the composition of natural hydrocarbon fluids, with only two main parameters: α and β. α sets the amount and distribution of heavy components (C_{10+}), whereas β is related to the methane content of the fluid. Physico-chemical properties of oils (density, liquid–vapor phase relations) are calculated by means of a modified Peng–Robinson equation of state (Peng and Robinson, 1976).

The (α–β) compositional model provides us with a simple way to graphically represent the composition of any hydrocarbon fluid. The (α–β) parameters have been calculated for several natural hydrocarbons from

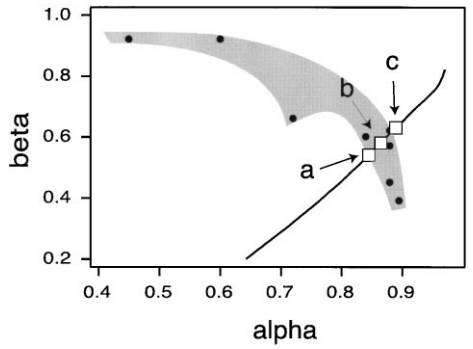

Fig. 4. The $\alpha-\beta$ diagram showing the $(\alpha-\beta)$ curve calculated by PIT for the inclusion of the Alwyn field. Three possible sets of $(\alpha-\beta)$ values in the main correlation field, called (a), (b), and (c), respectively, can be tested for this inclusion.

composition data and their $P-T$ bubble points. Values plotted in Fig. 3 show that a general correlation exists between the α and β parameters for natural oils. Numerous additional data from the Elf Aquitaine database (but not presented in Fig. 3) confirm this correlation.

An optimization procedure has been implemented in PIT in order to get the $(\alpha-\beta)$ compositional parameters, that best fit (F_v-T_h) data of the trapped oil (Fig. 1). PIT provides a set of possible values, represented by a curve in the $(\alpha-\beta)$ diagram. Intersection of this line with the main correlation, presented above, allows us to restrain the range of $(\alpha-\beta)$ values characterizing the fluid inclusion.

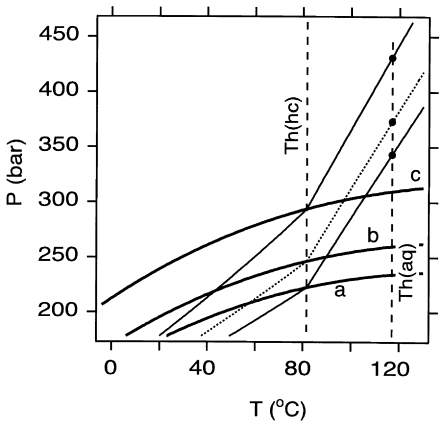

Fig. 5. The $P-T$ phase diagram, calculated by PIT for the three $(\alpha-\beta)$ sets, (a), (b), and (c).

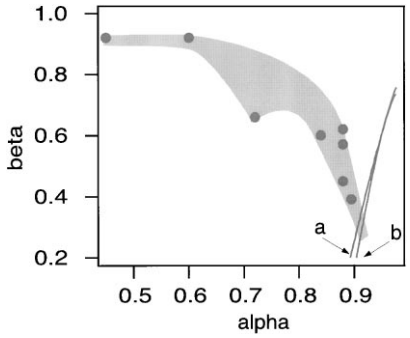

Fig. 6. The $\alpha-\beta$ diagram showing the $(\alpha-\beta)$ curves of oil inclusions (a) and (b) in fluorite.

3. Applications

A first application example of PIT is given here. Consider an oil fluid inclusion from the Alwyn field (North Sea) that homogenizes at $T_h = 81.6°C$ and presents a bubble filling degree (F_v) of 25.3% at 0°C. The $(\alpha-\beta)$ curve calculated by PIT is given in Fig. 4. It shows that the trapped oil is neither a light oil nor a heavy oil, but has a rather intermediate composition.

The $P-T$ phase diagrams and isochoric paths are calculated by PIT for the three sets, (a), (b) and (c), and drawn in Fig. 5. This oil inclusion is associated with aqueous fluid inclusions, which are supposed to be contemporaneous. Thus, the homogenization temperature of the H_2O-rich inclusion is assumed to be also the trapping temperature of oil fluid inclusions. Trapping pressures are simply estimated by reading the pressure value at the trapping temperature along the isochoric curves. In this example, values between 340 bar (case a) and 430 bar (case c) are obtained. The range is quite large ($\pm$50 bar), but the lower limit (case a: 340 bar) agrees well with present estimations of the past $P-T$ regime of the Alwyn field.

PIT can also give other useful indications on oil fluid inclusions. During its migration, oil can be altered by various processes: liquid–gas de-mixing, oils mixing, leaching by a gas or an aqueous solution, biodegradation, etc. All of these phenomena can be enregistered by oil fluid inclusions as they trap successive aliquots of migrating fluids. After entrapment, other processes can also alter the properties of oils (leakage, necking down, chemical reactions, etc.). Thus, it is common to observe very different (F_v-T_h)

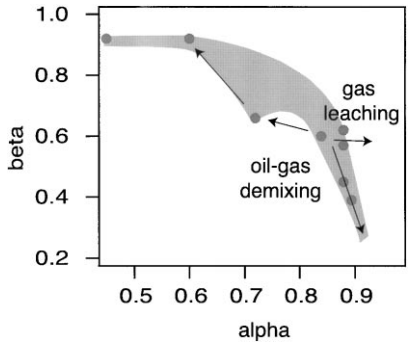

Fig. 7. ($\alpha-\beta$) diagram illustrating the effects of two main differentiation processes (liquid–gas immiscibility and gas leaching) on the ($\alpha-\beta$) parameters of hydrocarbons.

characteristics in a population of oil fluid inclusions in the same sample. PIT offers the possibility of analyzing and understanding the causes of these (F_v–T_h) differences.

Consider the case of two oil fluid inclusions (a) and (b) in fluorite, which present clearly distinct (F_v–T_h) characteristics. The first one homogenizes at 110.1°C and has an F_v of 9.5% at 20.1°C, whereas the second one homogenizes at 132.6°C and has an F_v of 13.4% at −18.4°C. These values suggest that these inclusions do not trap the same fluids. Fig. 6 shows us that the ($\alpha-\beta$) curves, calculated by PIT for these two inclusions, are almost coincident. It means that the same fluid, probably heavy oil, is trapped in these inclusions. The (F_v–T_h) characteristics are certainly produced by post-trapping deformations, a phenomenon that is not surprising since fluorite is known to deform plastically.

This makes it possible to detect other oil differentiation processes, which occur during oil migration. For example, the gas leaching of an immobile oil produces ($\alpha-\beta$) values aligned along a horizontal line in the ($\alpha-\beta$) diagram (Fig. 7): the α parameter increases, whereas the β parameter remains constant. Liquid–gas immiscibility (which can occur when the oil migrates toward shallower levels) generates more differentiated fluids. Residual oils, after de-mixing, have ($\alpha-\beta$) points which are aligned along an almost vertical curve: the α value increases slightly, whereas the β parameter decreases strongly. First de-mixed gasses are gas condensates and move progressively toward wet and dry gases.

4. Conclusions

One shortcoming of the VTFLINC software (Aplin et al., 1999) is that the user has to enter an initial oil composition to launch the calculations. As a consequence, the calculated solution by VTFLINC (i.e. the oil composition that closely matches the observed (F_v–T_h) characteristics of the fluid inclusion) clearly depends on the oil composition initially entered by the user. Such a procedure is obviously not satisfactory. PIT provides a solution to this problem: it proposes a compositional correlation, widely used and approved by oil engineers, and a practical graphical representation—the ($\alpha-\beta$) diagram for constraining composition estimations. Moreover, with this tool the user also has the possibility of identifying various differentiation processes that have affected petroleum in sedimentary basins.

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