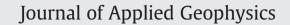
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Numerical modeling of thermal evolution in the contact aureole of a 0.9 m thick dolerite dike in the Jurassic siltstone section from Isle of Skye, Scotland

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ABSTRACT

In this study, we present a heat-transfer-model analysis of thermal evolution in the contact aureole of a 0.9 m thick dolerite dike in the Jurassic siltstone section from Isle of Skye, Scotland based on the constraints from the two types of vitrinite-reflectance geothermometers as well as geochemistry and burial history of host rocks. The predictions from the heat conduction models assuming the finite-time magma intrusion mechanism and pore-water volatilization can match well with both measured vitrinite reflectances and geological conditions of the host rocks. In the region where pore water volatilized and vitrinite reflectance rises with decreasing distance to the dike contact, the bomb geothermometer is consistent with the EASY%Ro model in validating the thermal evolution history of the host rocks, whereas it loses the function of temperature indicator out of the volatilization region. Possibly, the pore-water volatilization influenced the reliability of the bomb geothermometer. The computed total organic carbon contents based on the reconstructed thermal evolution history and the EASY%Ro model present the general agreement with the measured values, demonstrating the availability of the EASY%Ro model in indicating organic-matter transformation ratios at contact metamorphic conditions.

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1. Introduction

Heat transfer models offer an important tool for quantitatively evaluating the thermal effect of igneous intrusions on organic-rich host rocks in sedimentary basins (Aarnes et al., 2010; Barker et al., 1998; Delaney, 1987; Fjeldskaar et al., 2008; Galushkin, 1997; Jaeger, 1959; Jones et al., 2007; Monreal et al., 2009; Stewart et al., 2005; Wang, 2012; Wang and Song, 2012; Wang et al., 2007, 2010, 2011a,b). The assumptions about magma intrusion mechanisms and phase states of pore water may influence the model prediction significantly, and their uncertainties will result in an unreliable estimation of the thermal effect of igneous intrusions (Galushkin, 1997; Wang, 2012; Wang et al., 2011a). However, recent studies show that the magma intrusion mechanism and the phase state of pore water are still two controversial issues in the numerical modeling of heat transfer from igneous intrusions into host rocks (e.g. Aarnes et al., 2010; Fjeldskaar et al., 2008; Santos et al., 2009; Wang et al., 2007, 2008, 2011a,b). Therefore, it is necessary to further discuss the availability of different magma intrusion mechanism assumptions as well as the effect of different pore-water states based on some geological cases.

In addition, more than one type of vitrinite-reflectance geothermometers have been used to validate the thermal evolution history of the host rocks by calibrating the peak temperature (T_{peak}) or evaluating organic-matter maturation of host rocks (e.g. Barker et al., 1998; Bostick, 1971; Bostick and Pawlewicz, 1984; Sweeney and Burnham, 1990). These geothermometers are constructed based on theoretical analyses (e.g. Sweeney and Burnham, 1990) and laboratory experiments (e.g. Bostick, 1971; Bostick and Pawlewicz, 1984), or presented as a statistical relation between measured vitrinite reflectance (VRr) and the corresponding T_{peak} (e.g. Barker et al., 1998). In real contact metamorphic aureoles whose conditions are likely different from laboratory experiments and the normal burial diagenetic environments, the availability and applicability conditions of these geothermometers are not definite enough yet and also require further investigation based on real geological cases.

A 0.9 m thick dolerite dike intruded into the organic-rich Jurassic siltstone section from Isle of Skye, Scotland provides us with an opportunity to investigate all the uncertainties mentioned above. Bishop and Abbott (1993, 1995) analyzed geochemical characteristics of the sediments in the vicinity of this dike and measured their VR_r. Their work lays the basis for the model construction and validation. Galushkin (1997) modeled heat transfer from this dike into the host rocks, which provides sufficient parameters for our modeling. However, a few basic problems still remain unspecific. On one hand, the previous heat transfer modeling attempts was not, in general, successful. The uncertainties in the magma intrusion mechanism and the phase state of pore water contribute greatly to the unreliability of the heat-transfermodel analysis. By assuming the instantaneous magma intrusion mechanism, the prediction from the model used by Bishop and Abbott (1995) cannot match well with the measured VR_r. Galushkin' (1997) model,

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which assumed the finite-time magma intrusion mechanism, ignored the possibility of pore-water volatilization in shallow, water-saturated host rocks during cooling of magma and, hence, seems to deviate from real geological conditions. On the other hand, two types of VRr geothermometers are used to validate the used heat transfer models. The bomb geothermometer of Bostick and Pawlewicz (1984) was used in the work of Bishop and Abbott (1995), whereas the EASY%Ro model of Sweeney and Burnham (1990) was adopted by Galushkin (1997). No evidence indicates good agreement between these two geothermometers in calibrating the thermal evolution of the host rocks. Whether these two geothermometers are reliable to validate the thermal evolution history in the contact aureole of this 0.9 m thick dike is still unspecific.

In this study, we accordingly investigate the applicability of the heat transfer models assuming the different magma intrusion mechanisms and phase states of pore water to the 0.9 m thick dike from Isle of Skye, Scotland. Based on a comparison among the model prediction and the different types of VRr geothermometers, we also discuss the availability and consistency of these geothermometers in calibrating the thermal evolution history of the contact aureole of this dike. Finally, the deviation between the computed total organic carbon (TOC) of the host rocks by the model and the measured values is analyzed to demonstrate the capability of the EASY%Ro model in evaluating the transformation ratios of organic matter in real contact metamorphic environments.

2. Geologic setting

The Isle of Skye is located in the northwest of Scotland (Fig. 1). The coast of northwest Scotland was the site of intense Tertiary volcanic activities associated with the opening of the North Atlantic. Thick basalt lava flows overlay many of these Mesozoic basins. A schematic geological cross-section representing the structural disposition of these Mesozoic sedimentary basins is shown in Fig. 2. Consequently, igneous processes influenced the petroleum formation within basins (Bishop and Abbott, 1995). A 0.9 m thick Lower Eocene (about 53 Ma) dolerite dike was found to intrude the organic-rich Jurassic siltstone section from the Isle of Skye (Bishop and Abbott, 1995). The detailed geochemical characteristics of the host rocks in this section have been presented in the work of Bishop and Abbott (1993, 1995). Their analysis shows that the dike caused a significant carbon loss in the silty shale nearest to the intrusion (Fig. 3a). Maturation of organic matter in the contact metamorphic aureole of this dike is also strongly affected by the extreme heating of cooling magma, presenting extraordinary high VR_r values (Fig. 3b).

According to Galushkin (1997), 0.5 km thick siltstones in this section were deposited in the Toarcian and Aalenian stages of the Jurassic (187-173 Ma) and another 0.5 km thickness of siltstones were deposited from the Bajocian stage of the Middle Jurassic to the Lower Eocene (173–55.5 Ma). In terms of the background VR_r of the host rocks (~0.35%, Bishop and Abbott, 1995), Galushkin (1997) deduced that an interruption in sedimentation likely occurred from 55.5 Ma to the present time. Otherwise, the VR_r at the current burial depth (~640 m) should be higher than the measured value. The burial history of sedimentary formations proposed by Galushkin (1997) is shown in Fig. 4. Thus, the burial depth of the host rocks at the time of dike intrusion can be estimated to be approximately equal to the current value. In addition, Morton (1987) thought that the maximum burial depth experienced by the shales adjacent to this dike never exceeded 1 km. This is also consistent with Galushkin's (1997) estimate for the burial depth of the host rocks. The initial temperature of the host rocks at the intrusion moment of magma can be estimated to be approximately equal to 50 °C based on the burial history and the maximum burial depth of the host rocks (Bishop and Abbott, 1995).

3. Method

3.1. Heat transfer models

Similar to Bishop and Abbott (1995) and Galushkin (1997), we also adopt one-dimensional heat conduction models to describe the heat transfer from the Isle of Skye dolerite dike to its low-permeability organic-rich host rocks. A complete one-dimensional heat conduction model can be expressed as below (Wang et al., 2011a):

For the dike:

$$\frac{\partial}{\partial Z} \left(K_{\text{magma}} \cdot \frac{\partial T}{\partial Z} \right) = \frac{\partial \left(\rho_{\text{magma}} \cdot C_{\text{magma}} \cdot T \right)}{\partial t} + A_1. \tag{1}$$

For the host rocks:

$$\frac{\partial}{\partial Z} \left(K_{\text{host}} \cdot \frac{\partial T}{\partial Z} \right) = \frac{\partial}{\partial t} (\rho_{\text{host}} \cdot C_{\text{host}} \cdot T) + A_2 + [A_3].$$
⁽²⁾

Where *K* means the thermal conductivity; *C* is the specific heat; and ρ denotes the density. The subscripts, i.e. magma and host, represent magma and host rocks, respectively. A_1 is the latent crystallization heat of magma per unit of volume and time; A_2 and A_3 are the latent heat consumed by dehydration and decarbonation reactions of host rock matrix as well as pore-water volatilization per unit of volume and time, respectively. The computational methods of A_1 , A_2 , and A_3 have been introduced in the work of Wang et al. (2011a). The term A_3 in square brackets ([]) is optional and can be specified in terms of the geological conditions of the host rocks. It needs to be indicated that when pore-water volatilization is considered as a heat sink in the heat conduction model, such heat conduction model is named as the complex heat conduction model (Barker et al., 1998; Wang et al., 2007).

Pore-water volatilization usually needs to be accounted for when modeling the heat transfer from shallow, buried igneous intrusions to their host rocks (Jaeger, 1959; Santos et al., 2009; Wang et al., 2007, 2011a,b). In terms of the burial history of the Jurassic Isle of Skye siltstone section (Fig. 4), the host rocks of the 0.9 m thick dike could possibly have high porosity. If this is the case, pore-water volatilization could possibly influence the thermal evolution of the host rocks significantly and needs to be considered in the heat transfer modeling (Bishop and Abbott, 1995). Except for pore-water volatilization, the uncertainty in magma intrusion mechanisms can also have a notable influence on the model predictions (Galushkin, 1997; Wang, 2012). Usually, two types of magma intrusion mechanisms are assumed in the heat transfer modeling of igneous intrusions: 1) the instantaneous intrusion mechanism (e.g. Aarnes et al., 2010; Barker et al., 1998; Fjeldskaar et al., 2008; Jaeger, 1959; Santos et al., 2009; Wang et al., 2007), and 2) the finitetime intrusion mechanism (Galushkin, 1997; Wang, 2012; Wang et al., 2011a). In essence, the finite-time intrusion mechanism considers the flow duration and cooling of magma in the intrusion process of the dike. In terms of the different magma intrusion mechanisms and whether pore water volatilized during cooling of magma, the used heat conduction models of igneous intrusions in this study can be classified into four types (Table 1).

Furthermore, just as shown in Fig. 3b, near the dike contact, VR_r decreases with decreasing distance to the dike margin, whereas it generally increases with decreasing distance in the further host rocks. Some researchers also observed abnormally low VR_r near other igneous intrusions (e.g. Barker et al., 1998; Raymond and Murchison, 1988; Wang et al., 2007). Such reversals of VR_r can possibly be attributed to molecular disordering of the vitrinite at such high reflectance levels (Barker et al., 1998; Bishop and Abbott, 1995; Khorasani et al., 1990). The abnormal VR_r cannot be used to validate the thermal evolution history of the

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