Journal of Applied Geophysics 89 (2013) 134–140

Contents lists available at SciVerse ScienceDirect

Journal of Applied Geophysics

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

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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ARTICLE INFO

Article history:
Received 11 September 2012
Accepted 17 December 2012
Available online 23 December 2012

Keywords:
Igneous intrusion
Heat transfer model
Vitrinite reflectance
Peak temperature
Magma intrusion mechanism
Volatilization

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.

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-transfer-model 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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0926-9851/$ – see front matter
http://dx.doi.org/10.1016/j.jappgeo.2012.12.004

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:

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

For the host rocks:

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

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 finite-time 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

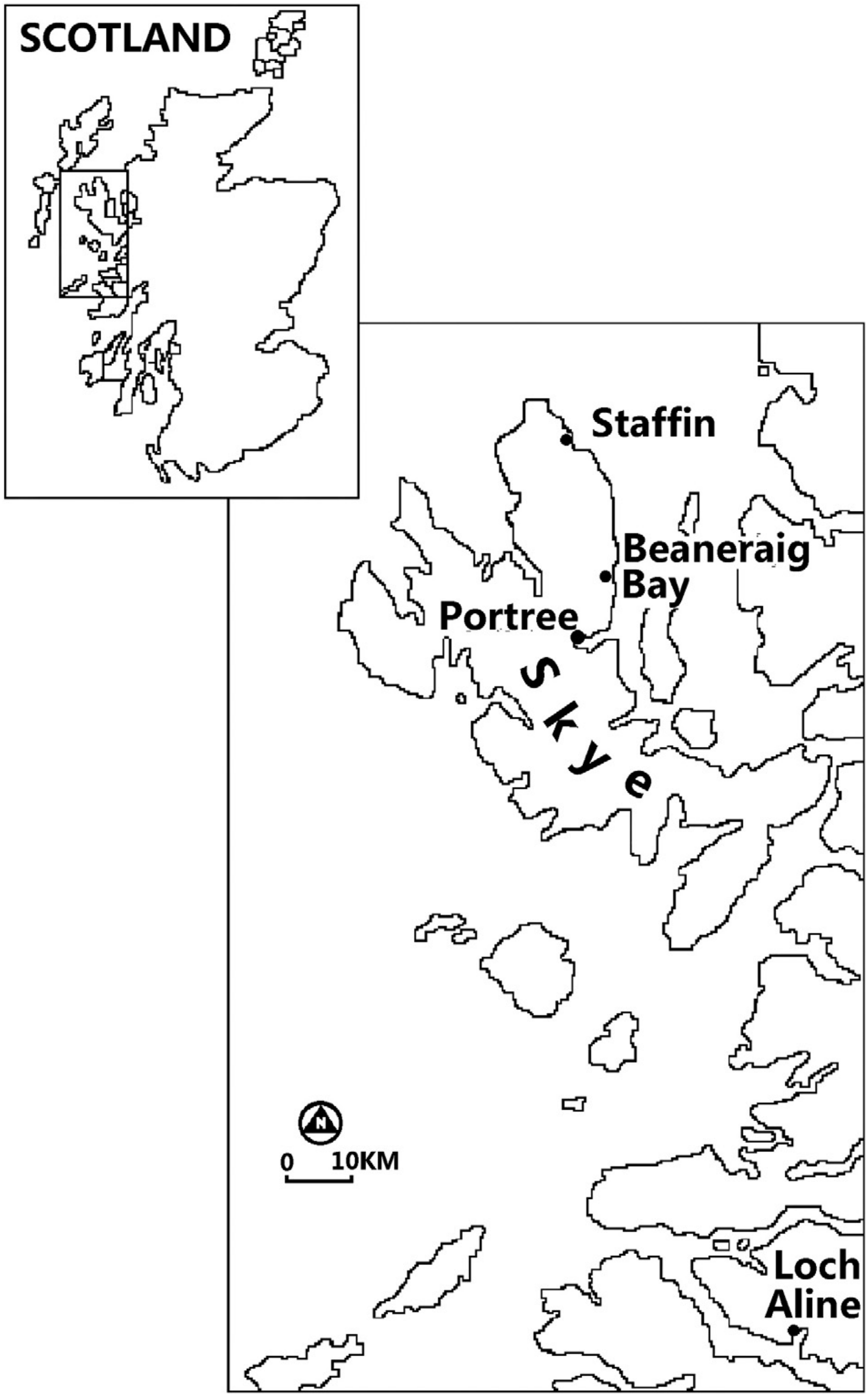

Fig. 1. Map of Isle of Skye, Scotland (modified after Bishop and Abbott, 1995).

host rocks. The unreliability of the used VR_r geothermometers in the reversal region will not be discussed in subsequent sections.

3.2. Model boundaries and parameters

Since the heat of an igneous dike is usually approximately symmetrically transferred into its both sides, one of two model boundaries can be located at the vertical central line of the dike. It is reasonably assumed that no heat flow passes through this boundary. Similar to Barker et al. (1998), the other model boundary is specified at the location with a distance (X) of five-times dike thickness (D) away from the dike margin (i.e. $X/D=5$). On this boundary, the temperature is assumed to remain constant during cooling of magma.

The values of most model parameters have been specified in the work of Galushkin (1997). The thermal conductivity and density of basic igneous intrusions are usually equal to 2.1 J m^{-1} s^{-1} $°C^{-1}$ and 2700 kg/m^3, respectively (Barker et al., 1998; Galushkin, 1997). The intrusion temperature of the dike in melting state is about 1100 °C (Galushkin, 1997). The specific heat of the dike is set as 1213 J/kg, which is equivalent to the specific heat of basic igneous

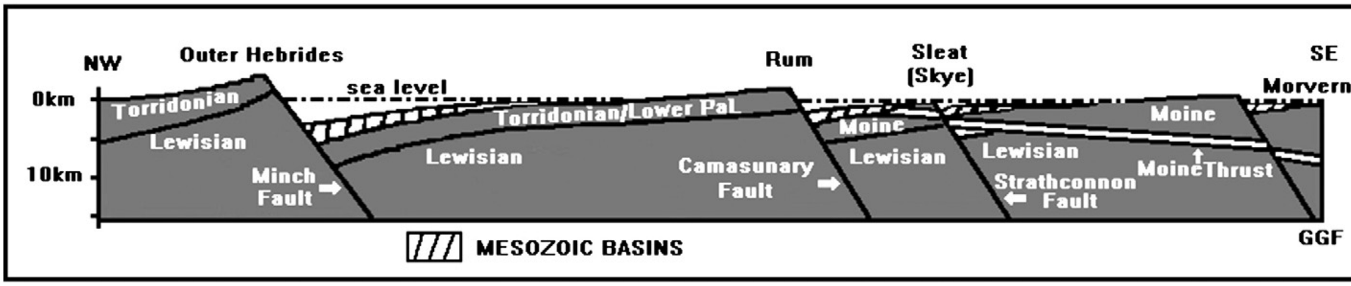

Fig. 2. Schematic Jurassic cross-section from the Outer Isles to the mainland SE of Skye, showing structural disposition of main Mesozoic sedimentary basins (Hesselbo and Coe, 2000).

intrusions at about 900 °C (Galushkin, 1997; Wang et al., 2010). Magma crystallization took place in a temperature range from 950 °C to 1150 °C, and the corresponding latent crystallization heat is equal to 376 kJ/kg (Galushkin, 1997).

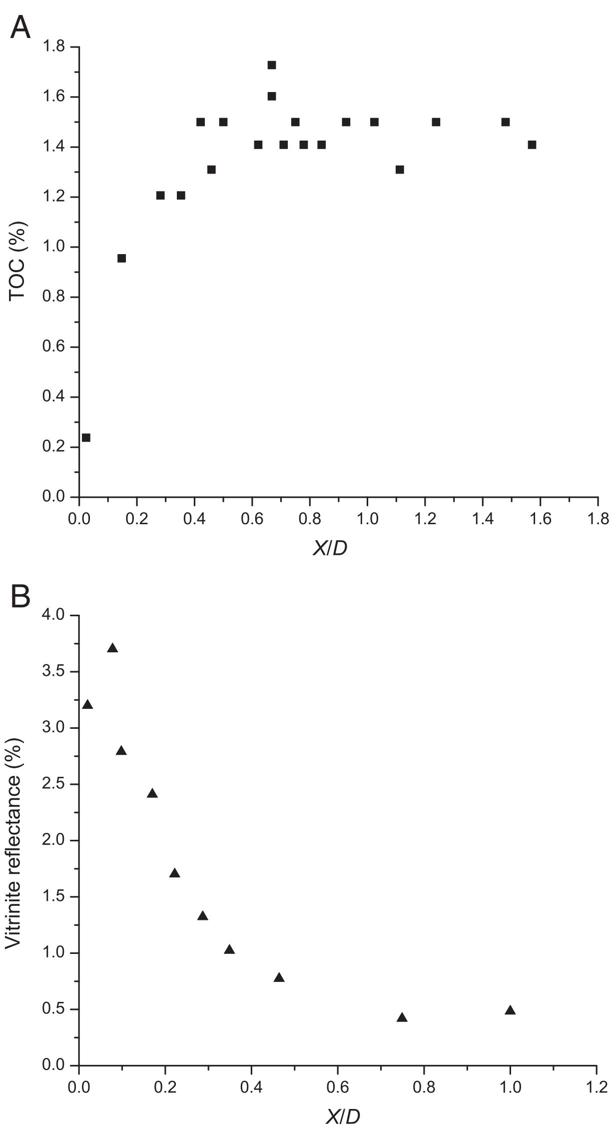

Fig. 3. Variation of (A) total organic carbon (TOC) and (B) vitrinite reflectance in the vicinity of a 0.9 m thick dolerite dike in the Jurassic siltstone section from Isle of Skye, Scotland with distance to dike margin (Bishop and Abbott, 1995). D means the dike thickness, and X denotes the distance from the dike margin to the host rocks.

At the burial depth of 640 m, the boiling point of pore water reaches about 300 °C, and its latent volatilization heat is approximately equal to 1398 kJ/kg. The porosity of the host rocks can be deduced to approach 0.45 in terms of the depth–porosity relationship of shales (Allen and Allen, 2005). However, 0.45 only represents the potential maximum porosity. Considering diagenetic modifications of the porosity, the real porosity of the host rocks will likely be <0.45. Thus, we also assumed 0.05 and 0.2 as the additional porosity options of the host rocks for the heat transfer models. According to Galushkin (1997), the latent heat of dehydration and decarbonation reactions of host rock matrix (pelite) reaches about 170 kJ/kg and the dehydration and decarbonation reactions took place approximately in a temperature range between 350 °C and 650 °C. The specific heat, the thermal conductivity and the density of the host rock matrix are approximately equal to 820 J/kg, 1.31 J m^{-1} s^{-1} $°C^{-1}$ and 2700 kg/m^3, respectively (Galushkin, 1997; Wang et al., 2007, 2011a). We calculated the total thermal conductivity and the total specific heat of the host rocks to be 1.0 J m^{-1} s^{-1} $°C^{-1}$ and 1582 J kg^{-1} $°C^{-1}$, respectively, based on the computational equations of Travis et al. (1991), Wohletz et al. (1999), Wang et al. (2007) and Wang et al. (2011a).

In the case of the finite-time magma intrusion mechanism, the temperature at the margin of the pre-cooled shell of the dike is set as 300 °C during formation of the dike (Galushkin, 1997). The time interval (t_0) during which the temperature at the dike axis increases from 300 °C to 1100 °C is usually uncertain. According to a statistics based on the case studies of Galushkin (1997), the ratio of t_0 to the total formation time of the dike lies in a range from 2:10 to 7:10. Although the used t_0 is possibly different for the different heat conduction models, the total formation time of the dike is assumed to be the same and equal to ~0.55 h.

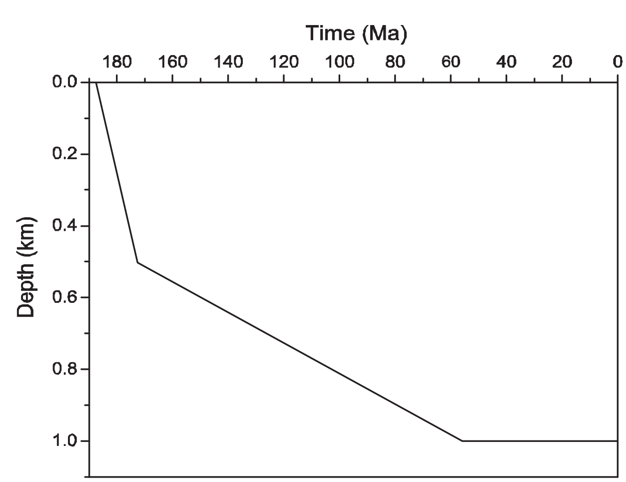

Fig. 4. Burial history of the Jurassic siltstone section of Isle of Skye, northwest Scotland (Galushkin, 1997).

Table 1
Four types of heat conduction models.

Type no.	Intrusion mechanism of magma	Pore-water volatilization	References
1	Instantaneous	Not considered	Barker et al. (1998), Fjeldskaar et al. (2008), Wang et al. (2008), Santos et al. (2009)
2	Instantaneous	Considered	Wang et al. (2007, 2011b)
3	Finite-time	Not considered	Galushkin (1997)
4	Finite-time	Considered	Wang et al. (2011a)

3.3. Computation of the peak temperature and organic-matter maturation of the host rocks

The T_{peak} can be obtained by computing the maximum temperature experienced by the host rocks during the cooling of magma based on the heat transfer model (Wang et al., 2010). Besides, the bomb geothermometer can also be used to estimate the T_{peak} of the host rocks (Bishop and Abbott, 1995). Bostick (1971) constructed the bomb geothermometer for igneous contact zones in sedimentary rocks using VR_r as a temperature indicator. This geothermometer was calibrated from laboratory experiments in which lignite in water was heated for a month in pressure bombs at specific temperatures up to 450 °C. Above 450 °C, the errors of the bomb geothermometer will become obvious, e.g., 40 °C at 500 °C and 100 °C at 600 °C (Bostick and Pawlewicz, 1984).

Maturation of organic matter in sedimentary rocks strongly depends on its thermal-evolution history and can be calculated based on the EASY%Ro model of Sweeney and Burnham (1990):

$$\text{EASY\%Ro} = \exp(3.7F - 1.6) \tag{3}$$

$$F = \sum_{i=1}^{20} f_i \cdot (1 - C_i/C_{0i}) = \sum_{i=1}^{20} f_i \cdot (1 - \exp(-I_i)) \tag{4}$$

$$I_i = \int_0^{t_1} A \cdot \exp(-E_i/(R \cdot T(t))) \cdot dt = \int_0^{t_2} A \cdot \exp(-E_i/(R \cdot T(t))) \cdot dt + \int_{t_2}^{t_1} A \cdot \exp(-E_i/(R \cdot T(t))) \cdot dt \tag{5}$$

where F is the transformation ratio for vitrinite reflectance; f_i represents the weight for the i_{th} reaction; A is the Arrhenius or frequency factor; E_i denotes the activation energy for the i_{th} reaction; R is the ideal gas constant; t means time; $T(t)$ is the temperature at the time t; t_1 is the final time; and t_2 means the time when magma intruded into its host rocks. The values of f_i, A, and E_i are obtained from Sweeney and Burnham (1990). I_i and F at any time during cooling of magma intrusions can be computed according to Braun and Burnham (1987). In this study, both the EASY%Ro model and the bomb geothermometer are used to calibrate the thermal evolution history of the host rocks.

4. Results and discussion

4.1. The applicability of different magma intrusion mechanisms and pore-water phase states to the used geological example

The VR_r and T_{peak} profiles of the host rocks predicted by the four types of heat conduction models (i.e. Types 1–4 in Table 1) are shown in Fig. 5. Just as shown in Fig. 5, the predictions from the heat conduction models assuming the instantaneous magma intrusion mechanism and ignoring pore-water volatilization largely exceed the calibrations by the two types of vitrinite-reflectance geothermometers. Under the assumption of the instantaneous magma intrusion mechanism, even if a large porosity is assumed for the host rocks, the predicted VR_r by the heat conduction model considering pore-water volatilization (i.e. Type 2 in Table 1) is still higher than the measurement value. Except for the magma intrusion mechanism, the intrusion temperature and the latent crystallization heat of magma are also important parameters for determining the total amount of heat of the dike and can accordingly influence the degree and extent of the thermal effect of the dike (Wang, 2012). In this study, the specified intrusion temperature (1100 °C) and the latent crystallization heat (376 kJ/kg) for the dike are lower than those (e.g. 1150 °C and 360 kJ/kg) used in some other case studies on basic igneous intrusions (Aarnes et al., 2010; Barker et al., 1998). Thus, the errors in these thermo-physical parameters of the dike cannot lead to the significant over-estimation of the thermal effect of the dike. Obviously, the models assuming the instantaneous intrusion mechanism (i.e. Types 1–2 in Table 1) do not represent natural conditions.

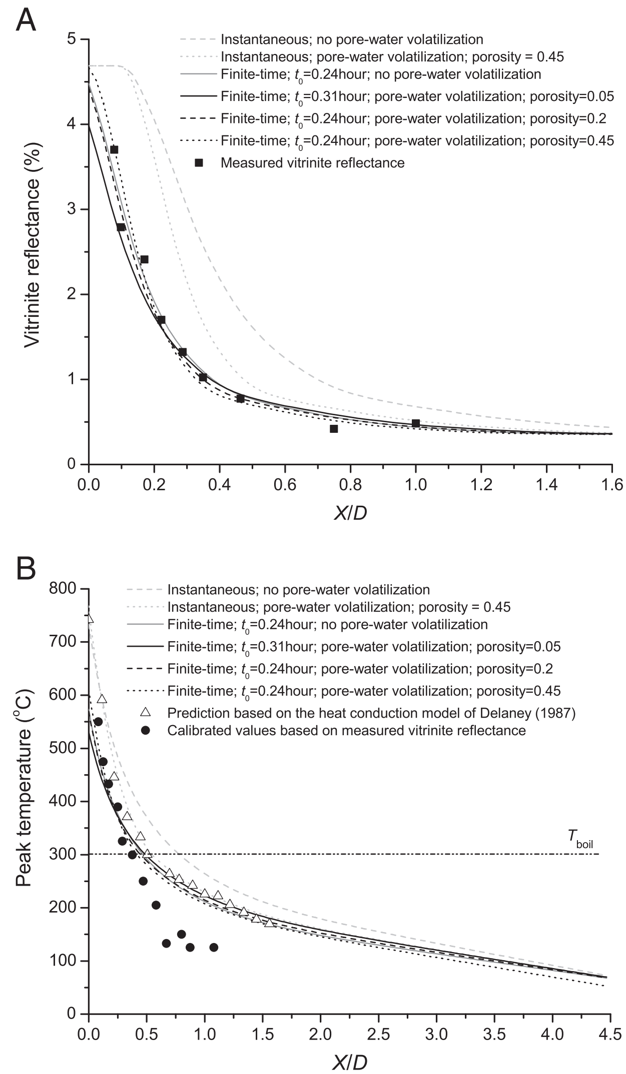

Fig. 5. Comparisons among heat-transfer-model predictions and calibrations by vitrinite-reflectance geothermometers. Two types of magma intrusion mechanisms (i.e. the instantaneous and finite-time intrusion mechanisms) are assumed for heat transfer models. Pore-water volatilization means that pore-water volatilization is allowed for in heat transfer models, whereas no pore-water volatilization denotes that pore-water volatilization is ignored in the model. The parameter, t_0, is only used by the finite-time intrusion mechanism and means the time interval during which the temperature at the dike axis increases from 300 °C to 1100 °C. T_{boil} is the boiling point of pore water, and $T_{background}$ denotes the temperature of the host rocks at the initial intrusion moment of magma. The meaning of X and D is the same as that in Fig. 3. The triangle symbols denote the computed peak temperature by the heat conduction model of Delaney (1987). The circle symbols represent the calibrated peak temperature based on the measured vitrinite reflectances and the bomb geothermometer of Bostick and Pawlewicz (1984). All measured vitrinite reflectances (the rectangle symbols) are from Bishop and Abbott (1995).

In addition, our simulation also shows that the predicted T_{peak} profile by the heat conduction model assuming the instantaneous intrusion mechanism and pore-water volatilization (i.e. Type 2 in Table 1) is approximately consistent with the computed one by Delaney (1987)'s model assuming the instantaneous magma intrusion mechanism. Bishop and Abbott (1995) thought that the overestimation of Delaney (1987)'s model of the spatial extent of the thermal effect might be mainly attributed to the fact that this model ignores thermal convection of the hydrothermal fluids in the host rocks. However, the hydrothermal convection in the host rocks can usually increase the spatial extent of the thermal effect of igneous intrusions (Wang et al., 2011a), thus resulting in a larger deviation between the model prediction and the T_{peak} estimated by the bomb geothermometer in the outer region of the contact aureole. Thus, it seems not to be the hydrothermal convection that leads to the overestimation of the heat transfer models of the spatial extent of the thermal effect of the dike.

As shown in Fig. 5, the VR_r predicted by the heat conduction model assuming the finite-time magma intrusion mechanism and ignoring pore-water volatilization (i.e. Type 3 in Table 1) matches well with the measurement value. According to the burial history, the host rocks could obtain a certain volume of pore water (Bishop and Abbott, 1995; Morton, 1987). The shallow burial depth of the host rocks implies that pore water could volatilize once its temperature exceeds its boiling point. Due to buoyancy, vapor produced by pore-water volatilization could escape upward and reduce the amount of heat in the aureole as a heat sink (Barker et al., 1998). Besides, the geochemical analysis indicates that the steam sourced from pore water in the host rocks likely played an important role in the carbon loss of the host rocks: the organic carbon in the host rocks at the contact reacted with steam, clay minerals being a potential catalyst, resulting in the formation of carbon monoxide and hydrogen (Bishop and Abbott, 1995). Thus, although the prediction of this type of model can match well with the measurement, it seems to deviate from the real geological condition.

Specifying the medium and large porosities for the host rocks (i.e. 0.2 and 0.45), the predicted VR_r by the heat conduction models assuming the finite-time magma intrusion mechanism and pore-water volatilization (i.e. Type 4 in Table 1) matches well with the measurement (i.e. the dashed and dotted black lines in Fig. 5). Under the assumption of the smaller porosity (i.e. 0.05), the VR_r profile computed by the same type of model (the solid black line in Fig. 5) may also basically match with the measurement value, but somewhat underestimates the thermal effect of the dike on the innermost host rocks in the aureole. As shown in Fig. 5, the volatilization of the larger volume of pore water can more significantly lower the thermal effect of the dike on the outer region of the contact aureole as a heat sink, but simultaneously tends to raise the VR_r and T_{peak} in the inner region by decreasing the thermal conductivity and the specific heat of the host rocks. By observing whether the model predictions can match well with the measurement values, we cannot confirm which porosity represents realistic conditions at the intrusion moment of the dike. Despite of the uncertainty in the porosity, if considering the burial history and geochemistry of the host rocks, the heat conduction model assuming the finite-time intrusion mechanism and pore-water volatilization likely approximately represents natural conditions.

4.2. The consistency of two vitrinite-reflectance geothermometers in calibrating thermal evolution history

In addition, the T_{peak} derived from the heat conduction model assuming the finite-time magma intrusion mechanism and pore-water volatilization also matches well with the calibration by the bomb geothermometer in the region where the T_{peak} of the host rocks exceeds the boiling point of pore water and VR_r rises with decreasing distance to the dike contact. This demonstrates that the bomb geothermometer and the EASY%Ro model are consistent in validating the thermal evolution history of the host rocks in such region. However, out of the volatilization region, the model prediction is obviously higher than the estimation based on the bomb geothermometer (Fig. 5). The estimated T_{peak} (~125 °C) based on the bomb geothermometer and the VR_r of the distal samples is almost invariant in the region of $X/D>0.65$. If the T_{peak} calibrated by the bomb geothermometer is accurate out of the volatilization region, 125 °C should approximately represent the background temperature of the host rocks unaffected by the heat of the dike. However, this temperature is obviously higher than the estimated initial temperature (~50 °C) of the host rocks at the intrusion moment of the dike and, hence, seems unrealistic. Bostick and Pawlewicz (1984) thought that the pressure is the main factor influencing the availability of the bomb geothermometer and that the bomb geothermometer is probably more accurate in the high-pressure environment. However, in terms of the burial history, the host rocks of the 0.9 m thick dike only correspond to the formation pressure of less than 10 MPa, far below the pressure of the high-pressure bomb experiment. The model prediction shows that in the host rocks where pore water volatilized, the bomb geothermometer is still reliable to calibrate the T_{peak}. This demonstrates that pressure might have no obvious influence on the availability of the bomb geothermometer. In addition, according to Barker et al. (1998), the generation of vapor or supercritical fluids can change vitrinite evolution reactions. The comparison between the calibrated T_{peak} by the bomb geothermometer and the heat-transfer-model prediction shows that the reliability of the bomb geothermometer seems to be influenced by the pore-water state. Unlike the T_{peak}–VR_r relationship proposed by Barker et al. (1998), which is usually only reliable in the region where pore water did not volatilize or was not converted into the supercritical state, the bomb geothermometer might be more applicable in the volatilization zone of pore water.

4.3. The reliability of the EASY%Ro model at contact metamorphic conditions

Some researchers used the EASY%Ro model to evaluate the transformation ratio of organic matter in the sediments (e.g. Aarnes et al., 2010; Fjeldskaar et al., 2008; Galushkin, 1997; Wang et al., 2011a). However, no studies have been conducted to test or prove the availability and accuracy of the EASY%Ro model at contact metamorphic conditions. The measured VR_r of the sediments furthest from the dike is about 0.35%, only corresponding to a 15% transformation ratio of the original organic matter in the host rocks based on the EASY%Ro model. According to Bishop and Abbott (1995), the sediments furthest from the dike have a TOC of *ca.* 1.5%. Thus, the initial TOC of the host rocks at the beginning of sedimentation can be deduced to reach ~1.77%. The computed TOC based on the EASY%Ro model and the reconstructed thermal evolution history by the heat conduction models, assuming the finite-time intrusion mechanism and pore-water volatilization, shows the general agreement with the measured values (Fig. 6). This demonstrates the availability of the EASY%Ro model at contact metamorphic conditions.

5. Conclusions

Based on the heat-transfer-model analysis of the thermal evolution in the contact aureole of a 0.9 m thick dolerite dike in the Jurassic siltstone section from Isle of Skye, Scotland, the following conclusions can be made:

(1) If assuming that magma was instantaneously intruded into sedimentary formations, organic-matter maturation and the peak temperature of the host rocks predicted by the heat conduction models are obviously higher than the estimates derived from the two different types of vitrinite-reflectance geothermometers: the EASY%Ro model of Sweeney and Burnham (1990) and the bomb geothermometer of Bostick (1971). The predictions from

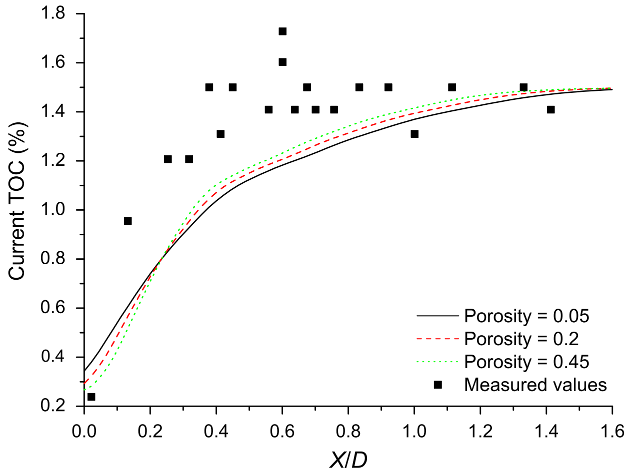

Fig. 6. A comparison between the predicted total organic carbon (TOC) by the heat conduction models of the finite-time magma intrusion mechanism and measured values. These models assume pore-water volatilization and different porosities for the host rocks. The meaning of *X* and *D* is the same as that in Fig. 3.

the heat conduction models assuming the finite-time magma intrusion mechanism can match well with the calibrations of these two types of vitrinite-reflectance geothermometers. Considering the burial history and geochemistry of the host rocks, the heat conduction model assuming pore-water volatilization and the finite-time magma intrusion mechanism most likely represents natural conditions.

(2) In the region where pore water volatilized and VR_r 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. Out of this region, the bomb geothermometer loses the function of temperature indicator. It might be the pore-water volatilization that influenced the reliability of this geothermometer.

(3) The computed total organic carbon based on the EASY%Ro model and the reconstructed thermal evolution history by the heat conduction model assuming the finite-time magma intrusion mechanism and pore-water volatilization presents the general agreement with the measured values. This demonstrates that the EASY%Ro model is a good indication of transformation ratios of organic matter at contact metamorphic conditions.

Acknowledgment

This work was financially supported by the National Science Foundation of China (no. 41004031), the 863 program (nos. 2008AA062303 and 2009AA063402), the 973 program (Nos. 2009CB219507 and 2011CB707304), the Ph.D. Programs Foundation of Ministry of Education of China (no. 20100041120039) and the Fundamental Research Funds for the Central Universities (no. DUT12JN13).

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