MagmaHeatNS1D: One-dimensional visualization numerical simulator for computing thermal evolution in a contact metamorphic aureole

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A B S T R A C T

MagmaHeatNS1D is an IDL (Interactive Data Language) program that is aimed at numerically modeling heat transfer from an igneous intrusion to its host rocks and providing important thermal state information for minerals and organic matters in a contact aureole. It can be used to trace temperature time series, computing the peak temperature, and evaluating organic-matter maturation in a contact aureole. The theoretical basis of the program is a complete one-dimensional heat transfer model, and, hence, the program can allow for numerous potential influencing factors on the heat transfer, involving magma crystallization, volatilization and the supercritical state of pore water, dehydration and decarbonation reactions of host rock matrix, instantaneous and finite-time magma intrusion mechanisms, and hydrothermal convection in host rocks. This ensures that the program can be applicable to study different igneous intrusions in various geological conditions. MagmaHeatNS1D features a graphical user interface for controlling program execution, displaying real-time results, outputting final results, and opening secondary windows which serve to input the model parameters. MagmaHeatNS1D can be used in an intuitive framework for educational and research purposes.

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1. Introduction

One-dimensional heat transfer models have been successfully applied in numerous case studies on the thermal effect of igneous intrusions on host rocks and are popular quantitative tools (e.g., Bostick and Pawléwicz, 1984; Delaney, 1988; Bishop and Abbott, 1995; Gvirtzman and Garfunkel, 1996; Galushkin, 1997; Barker et al., 1998; Stewart et al., 2005; Wang et al., 2007, 2010, 2011, 2012; Santos et al., 2009; Wang, 2012; Wang and Song, 2012). Recent advances in theoretical modeling have largely improved the capability of these one-dimensional models for representing natural conditions (Wang et al., 2010, 2012). A complete one-dimensional heat transfer model of igneous intrusions can implement conductive and convective heat-transfer modes, considering the supercritical state of pore water, and include several heat sinks and sources such as pore-water volatilization, magma crystallization, and dehydration and decarbonation of host rock matrix (Wang et al., 2011; Wang, 2012).

Usually, the developed numerical simulation programs are designed only for specific case studies (Galushkin, 1997; Barker et al., 1998; Wang et al., 2007; Santos et al., 2009). Because igneous intrusions and their host rocks in different contact aureoles have differing geological conditions, the heat transfer modeling for these aureoles has to be separately dealt with and distinguishably treated. Besides, the one-dimensional heat transfer model may be used to obtain various types of information about the thermal state of a contact aureole such as the contact temperature (Stewart et al., 2005; Wang et al., 2008) and the peak temperature (; Santos et al., 2009; ). Further, if the reconstructed thermal evolution history by the model is combined with the EASY%Ro model of Sweeney and Burnham (1990), the model will also be capable of evaluating organic-matter maturation of host rocks (Galushkin, 1997; Wang et al., 2011). In case studies of contact aureoles, different types of model outputs (e.g., the peak temperature, organic-matter maturation, and vitrinite reflectance) could possibly be required, depending on the research objectives and purpose of the modelers. Thus, the numerical simulation program, which is used to study a certain contact aureole for specific purpose, cannot often be used to study other examples of igneous intrusion and, hence, loses universality.

How to design a numerical simulation platform for the analysis of thermal state of a contact metamorphic aureole, which can simultaneously be used to study contact aureoles occurring with different geological conditions, is an important issue. To date, no such numerical simulation platform has been released...
in an intuitive framework for educational and research purposes. A numerical simulator called MagmaHeatNS1D has recently been developed to fill this gap. In this paper, a description of theory, function, and design method of this simulator will be presented in detail.

2. Theoretical models used in MagmaHeatNS1D

2.1. One-dimensional heat transfer models of igneous intrusions

The shape of many igneous intrusions is regular, dike-like or sill-like, and their length is usually much larger than their thickness (Jaeger, 1959; Turcotte and Schubert, 1982; Wang et al., 2007). For such intrusions, one-dimensional heat-transfer modeling can give a realistic estimate of their thermal cooling, with a significant reduction of computational cost and algorithm complexity (Fjeldskaar et al., 2008; Aarnes et al., 2010). Ignoring thermal convection in intrusive magma and the heat removed by escaping volatiles, a complete one-dimensional heat transfer model governing the temporal (t) and spatial (Z) variations of the temperature (T) in a contact aureole can be expressed as follows (Wang et al., 2011):

For a magma intrusion

\[
\frac{\partial}{\partial Z} \left( \frac{K_{magma} \partial T}{\partial Z} \right) = \rho_{magma} \frac{L_c}{T_{c1} - T_{c2}} \frac{\partial T}{\partial t} + \frac{\partial}{\partial t} \left( \rho_{magma} C_{magma} T \right) \tag{1}
\]

For host rocks

\[
\frac{\partial}{\partial Z} \left( (1 + Nu)K_{host} \frac{\partial T}{\partial Z} \right) = \frac{\partial}{\partial t} \left( \rho_{host} C_{host} T \right) + \left[ \frac{(1 - \phi) \rho_{matrix} L_c T_{c1} - T_{c2}}{\partial t} \right] + \left[ \frac{(1 - \phi) \rho_{water} \phi C_{water} \partial T}{\partial t} \right] \tag{2}
\]

The meaning of the notations in Eqs. (1) and (2) and all following equations is listed in Table 1. The terms in square brackets of Eq. (2) are optional and need to be specified in terms of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusive magma lies outside its solidification temperature range of different geological conditions. When the temperature of intrusiv

3. Overview of the MagmaHeatNS1D program

3.1. General features

MagmaHeatNS1D can be used to compute temperature evolution and organic-matter maturation in the contact aureole of an igneous intrusion with a regular shape, such as a dike or a sill. MagmaHeatNS1D is coded using IDL 6.4 (Interactive Data Language). It features a main graphical user interface (GUI) for controlling program execution, displaying real-time results, outputting final results and opening secondary windows (Fig. 1) which are used to input all the model parameters (Figs. 2–6).

3.2. Specifications of model boundaries and initial conditions

The Time Parameters window is used to enter time-related parameters, including the total duration of magma cooling, the time step for the finite difference scheme, and a pause time point (Fig. 2). If the numerical computation of the program indicates that cooling of intrusive magma lasts up to the pause time point, the program will pause running and wait for the user to examine and output the results. Once a new pause time point is re-set, the program will continue to run until the new pause time point is reached.

The space-related parameters are specified in the Space Parameters window (Fig. 3). The spatial range of the model domain is set by entering its start and end points. Using the Magma Zone text boxes allows input of the initial locations of two margins of intrusive magma. The magma zone, together with the whole model domain, will be then displayed inside the Domain widget in the middle of the window if the cursor is moved in the Domain widget. A pair of tick boxes are created to specify the type of two model boundaries (i.e., the upper and lower boundaries of the model domain appearing in the Domain widget). If the tick box is selected, the temperature at the corresponding boundary will remain invariant during cooling of magma (i.e., Dirichlet boundary condition), or else no heat flow is assumed to pass through this boundary (i.e., Neumann boundary condition). In the MagmaHeatNS1D program, the initial temperature of host rocks is computed in terms of the ground surface temperature, the geothermal gradient, and the burial depth. The computed initial temperature profile of host rocks can be shown in the Initial Geothermal Profile draw widget. In particular, the program allows the user to assume one of two types of intrusion mechanisms of magma for their models: the instantaneous intrusion mechanism (e.g. Jaeger, 1959; Barker et al., 1998; Santos et al., 2009) or the finite-time intrusion mechanism (e.g. Galushkin, 1997; Wang et al., 2012). The latter can be approximately described as — the temperature at the axis of a magma intrusion T_{axi} increases at a time interval t_{axis} from a relatively low initial temperature T_{magma0} to the temperature of melted magma T_{magma1} at a steady rate, and subsequently T_{axi} remains equal to T_{magma1} at a time interval t_{axis2} until the complete