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Numerical Modeling of the Hydrothermal Metallogenic Mechanism Associated with the Ergu Pb-Zn Deposit, Heilongjiang, China: An Example of Pore-Fluid Convection Controlled Mineralization

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Abstract: Skarn-hosted deposits are commonly recognized as the consequence of magma intrusion within the Earth’s upper crust. The Ergu Pb-Zn deposit can be regarded as a typical skarn-hosted deposit in the hydrothermal ore-forming system within the central Lesser Xing’an Range (LXR), Heilongjiang, China. Although extensive studies were conducted to understand the ore-forming system associated with the Ergu Pb-Zn deposit through using the traditional geoscience methods, the ore-forming process involved in this deposit has not been justified in a strictly scientific manner to date. In this paper, the hydrothermal ore-forming process of the Ergu Pb-Zn deposit is computationally simulated through using the dual length-scale approach associated with the finite element method (FEM). The related computational simulation results have demonstrated that: (1) the pore-fluid convection provides continuous ore-forming fluid and material sources for the Ergu Pb-Zn deposit at the quartz-Pb-Zn sulfide stage; (2) the convective flow of the pore fluid is the main dynamic mechanism, which controls the temperature, chemical species and pore-fluid velocity distributions in the Ergu Pb-Zn deposit; (3) the localized structure plays a key role in controlling the localized pore-fluid flow pattern, which can further control the location and formation of the orebody grade in the Ergu Pb-Zn deposit; (4) the dual length-scale approach associated with the FEM is very useful in dealing with the computational simulation of the hydrothermal ore-forming mechanism involved in the Ergu Pb-Zn deposit.

Keywords: dual length-scale; metallogenic process; Ergu deposit; convective pore-fluid flow; mineralization rate

1. Introduction

The Lesser Xing’an Range (LXR) is located in the eastern part of the Central Asian Orogenic Belt. It is one of the areas with well-endowed porphyry-skarn-epithermal Mo-Au-Fe-Cu-Pb-Zn polymetallic deposits in China [1–3]. It has been known that the Ergu Pb-Zn deposit can be considered as a representative skarn-hosted deposit in the central LXR. The existing investigations indicated that the Ergu Pb-Zn deposit can be used to determine the constraints, which may be imposed by a magma intrusion on the formation of a skarn-hosted polymetallic deposit. This means that not only does the study of the Ergu Pb-Zn deposit have great economic value, but it is also beneficial for revealing the ore-forming mechanism and resource potential of precious metals in the central LXR, Northeast China [3–5]. Therefore, the ore-forming mechanism of the Ergu Pb-Zn deposit has been extensively studied [3–10], and a brief summary of the main outcomes from the previous studies can be described as follows: (1) the structures and strata of the Ergu ore district were investigated, so that the related information is available for designing the geological model of the Ergu Pb-Zn deposit; (2) the alteration and mineralization characteristics of
the sphalerite and galena associated with the Ergu Pb-Zn deposit were determined, so that it is believed that the Ergu Pb-Zn deposit is formed at the quartz-Pb-Zn sulfide stage; (3) the stable isotopes, fluid inclusions and trace elements in the Ergu Pb-Zn deposit were studied, so that it is evidenced that the ore-forming fluid in the Ergu Pb-Zn deposit was mainly derived from the mixture of deep magmatic hydrothermal fluid and atmospheric precipitation at the quartz-Pb-Zn sulfide stage; (4) the Ergu Pb-Zn deposit can be best classified as a polymetallic skarn-hosted deposit, where the mineralization associated with the solidified magma occurred during the Early Jurassic; (5) the formation of the Ergu Pb-Zn deposit was structurally related to the subduction of the Early Jurassic Paleo-Pacific plate beneath Eurasia [6,11,12]; (6) the geologically stable period is very long, which can amount to over 20 million years after the intruded magma was completely solidified and cooled [13,14]. This means that according to the main outcomes from the previous studies, especially those mentioned in items (4) and (6) above, the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit could reach a steady state or a quasi-steady state after the intruded magma was completely solidified and cooled. Therefore, the main purpose of this study is to investigate the ore-forming process of the Ergu Pb-Zn deposit during such a long geologically stable period after the intruded magma was completely solidified and cooled. For this reason, the transient process associated with the magma solidification and cooling [15–18] is not considered in this study, although it deserves consideration in future research. This implies that the work presented in this study has a limited application scope, because it is only valid for the specific situation that is established on the bases of a steady-state or a quasi-steady-state hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit.

Nevertheless, due to the complicated ore-forming process associated with the Ergu Pb-Zn deposit, some key issues involved in this deposit still need to be resolved. For example, (1) where does the large amount of hydrothermal fluid, which is necessary for forming such a huge deposit, come from? (2) What were the spatiotemporal evolution characteristics of the temperature, velocity of pore-fluid and velocity of pore-fluid in the ore-forming system? (3) What was the effect of the sulfate reduction at the quartz-Pb-Zn sulfide stage of mineralization during the ore-forming fluid mixing? (4) What was the effect of nonlinearly coupled physical and chemical fields on mineralization? (5) What was the post-cooling influence of the solidified magma and tectonic faults on the orebody distribution in the ore-forming system? Obviously, these five fundamental questions involved in the formation of the Ergu Pb-Zn deposit need to be answered through considering the controlling dynamic processes and mechanisms in a strictly scientific manner [19–29].

As one of the most-encountered geological phenomena, mineralization within the Earth’s upper crust was extensively observed and investigated since ancient times. Although the traditional geoscience method is commonly used to describe the observed mineralization phenomena, it cannot be used to explain, in a strictly scientific manner, how and why the observed ore deposits formed where they are located, because the controlling dynamic processes involved in the mineralization and orebody formation are not considered in the traditional geoscience method [19,30,31]. In order to address this fundamental issue, the computational simulation method, which is closely associated with the emerging computational geosciences, has been developed and used in recent years [19–29,31,32]. Compared with the traditional geoscience method, the specific characteristics of the computational simulation method include the following four aspects. First, specific physical processes can be accurately taken into account in the computational simulation method. For instance, the pore-fluid flow can be described using Darcy’s law, while the mass flux associated with solute diffusion and the heat flux associated with heat conduction can be, respectively, described using Fick’s law and Fourier’s law. Second, three fundamental scientific principles in nature, such as mass conservation, energy conservation and momentum conservation, can be strictly satisfied in the considered ore-forming system. Third, mathematical governing equations (MGEs) can be derived and used for describing the controlling dynamic processes involved in the mineralization and orebody formation
associated with the considered ore-forming system. Fourth, advanced computational algorithms can be developed and used for solving the MGEs associated with the considered ore-forming system. Due to the aforementioned characteristics, computational simulation methods have been broadly used for solving many different types of problems in the field of geosciences [19–29,31–33]. Therefore, the computational simulation method is naturally chosen as a research tool in this study.

2. The Geological Setting of the Ergu Pb-Zn Deposit

2.1. Geological Background

As stated in the previous study [3], the Ergu Pb-Zn deposit is located in the central LXR (Figure 1), which straddles the North China Craton, Pacific Plate and Siberian Craton. In addition, the central LXR is also separated from these blocks by the Jiayin-Mudanjiang and Hegenshan-Heihe faults. It was reported that the LXR has a complex tectonic history, which contains the typical events, such as the Cenozoic supracrustal faulting, the Mesozoic subduction influence of the Paleo-Pacific Plate and the Paleo-Asian Ocean evolution [34–36]. Consequently, there are a large number of structural, magmatic and mineralization events in the LXR.

Figure 1. The regional geological map: (A) The location of Northeast China with respect to the main tectonic units of China and Russia. “A” and “M” represent the Altaids and Manchrids (modified from [2]). (B) Tectonic sketch maps of Northeast China (modified from [2]). (C) The geological map of the Lesser Xing’an range (modified from [1–3]).

The previous study [5] also stated that: “the stratigraphy of this region is dominated by the gold-bearing silicoferrite of the Dongfengshan Formation (801–821 Ma) [37] and the overlying Cambrian–Ordovician neritic facies clastic rocks (about 500 Ma) [38], Permian terrigenous clastic-carbonate formations [6], Mesozoic continental volcanic rocks (including two stages: 190–170 Ma and 130–105 Ma) and Palaeogene fluvial and lacustrine clastic sedimentary rocks. The exposed strata in the mining area are typically the lower Cambrian...
Qianshan and Laodaogoumiao Formations, which consist of crystalline limestone and marble, silt slate and hornstone, respectively. The Permian Wudaoling Formation and Quaternary are also well developed in the mining area, consisting of dacitic tuffaceous lava and alluvial sediments, respectively. In addition, the unit closely related to mineralization is the Qianshan Formation, while the early Palaeozoic strata in the mining area were destroyed by the influence of magmatic and structural activity [6].

The dominant regional structures are oriented either in the northeast direction or in the nearly north–south direction and include the Dunhua–Mishan fault, Yitong–Yilan fault and Jiayin–Mudanjiang fault. It is believed that the distributions of igneous rocks and deposits were controlled at large by these dominant regional structures [6,8,39–44]. In the LXR, the representative deposits are (1) Cuiling, Gaosongshan, Luming and Huojihe porphyry Mo deposits; (2) Gaosongshan, Yongxin and Dong’anm epithermal gold deposits; and (3) Ergu, Baoshan and Cuihongshan skarn-hosted deposits. In addition, the Ergu-Xulaojiugou in anticline, which is oriented in the north–south direction, is another main structure to control the distribution of orebodies in the mining area [3].

It was reported that the voluminous Phanerozoic granitoids were found in the LXR [45,46], which experienced the following six stages of magmatism [2,47–52]: (1) Middle Cambrian–Late Ordovician (508–450 Ma); (2) Middle–Late Permian (266–252 Ma); (3) Early Middle Triassic (244–231 Ma); (4) Late Triassic (222–200 Ma); (5) Early Jurassic (186–175 Ma); and (6) Early Cretaceous (154–101 Ma). In particular, the Late Triassic and Early Jurassic granites are the most common and closely related to the skarn-hosted deposits in the LXR [13,14].

2.2. Metallogenic Characteristics

As stated in the previous study [5], a total of 21 valuable orebodies were discovered. These valuable orebodies have lenticular, veined or cystiform shapes. The lengths of them vary from 30 m to 887 m, while the widths of them vary from 0.92 m to 13.9 m [3]. Based on the geological characteristics [3,4], it is believed that the locations of these orebodies are clearly controlled by the associated structures. Consequently, these orebodies show wavy distributions in the cross section. In particular, they can be found in the outer, middle and inner zones of the contact zone, which is located between the limestone rocks and granodiorite of the lower Cambrian Qianshan Formation (Figure 2a). It was also observed that when the above-mentioned contact zone displays the shapes of curves or a shallower dip, there is an obvious increase in the thickness of the orebody. The sizes of the orebodies generated within the contact zone vary from 1 m to 28 m. These orebodies are mainly enriched in Fe and Cu. However, the sizes of the orebodies generated far from the intruded granodiorite vary from 15 m to 87 m. These orebodies are mainly enriched in Pb and Zn.

According to a series of the previous studies [3–10], there are two periods involved in the ore-forming process. The first is a skarn forming period (i.e., period I), while the second is a quartz-sulfide period (i.e., period II). These two periods contain the following six mineralization stages [3]: a prograde skarn forming stage (i.e., stage I1), a retrograde skarn forming stage (i.e., stage I2), an oxide stage (i.e., stage I3), a quartz-Fe-Cu sulfide stage (i.e., stage I1), a quartz-Pb-Zn sulfide stage (i.e., stage II2) and a quartz-carbonate stage (i.e., stage III). This means that there are three stages in each period. In stage I1, a large number of anhydrous silicate minerals, such as the garnet and diopside formed in the endoskarn, are distributed within the retrograde skarn. In stage I2, the hydrous alteration minerals, such as chlorite, hornblende, epidote, actinolite and a small amount of magnetite, are extensively formed. In stage I3, a large amount of magnetite, including lesser amounts of molybdenite, pyrrhotite and quartz, is predominantly generated. Particularly, the formations of orebodies at this stage primarily take place within the fractures between the exoskarn and endoskarn. In stage I1, which is the ore-forming stage of the Fe-Cu orebodies, the formations of orebodies are primarily in the form of veins or veinlets, which are disseminated and generated as the structural protrusions within the exoskarn. In stage I2, which is the ore-forming stage of Pb–Zn orebodies, the formations of orebodies are
mostly in the form of net veins and veins occurring in the exoskarn. In this study, only the formation of galena at this stage is considered; although, the formations of other precious metals (e.g., Fe and Cu) in the other stage deserves consideration in future research. In stage II3, a large amount of calcite, fluorite, quartz and a small amount of pyrite and galena are primarily formed in the exoskarn.

2.3. Basic Questions Associated with Establishing Computational Models for Simulating the Ergu Pb-Zn Deposit

It is necessary to answer the following five basic questions before the computational simulation is used for studying the controlling ore-forming processes of a hydrothermal deposit [19–23,53]: (1) What were the architecture and material distribution characteristics of the total mineralizing system? (2) What was the geodynamic history leading to the evolution of temperature, pore-fluid pressure and pore-fluid velocity distributions? (3) What were the chemical and physical characteristics of the pore fluids involved in the system? (4) What were the mechanisms to drive the pore-fluid flow? (5) What were the processes and mechanisms involved in the metal dissolution, metal transport and metal precipitation?

To answer these five questions, a large number of geophysical and geochemical studies related to the Ergu Pb-Zn deposit have been carried out [3–7,50]. Based on the review of the outcomes from these geophysical and geochemical investigations, the above five questions can be answered as follows: (1) Through considering the data of geology, geophysics and geochemistry, it is believed that the distribution of the Ergu Pb-Zn deposit was controlled by both the granite body and the tectonic faults in the limestone strata. (2) Through referring to the tectonic background [5], it is believed that the magmatism and mineralization of
the Ergu Pb-Zn deposit were likely related to the magmatic arc system of the continental margin in eastern China where the Palaeo-Pacific Plate was subducting beneath Eurasia in the Mesozoic (Figure 2b). (3) From the stable isotope analysis, it is believed that the ore-forming fluid in the Ergu Pb-Zn deposit was mainly derived from the mixture of deep magmatic hydrothermal fluid and atmospheric precipitation in stage II2. In the migration and evolution processes of the ore-forming fluid, the seawater sulfate may contribute part of sulfur through a thermochemical reduction. (4) According to the analysis of metallocenic characteristics, it is believed that a temperature-triggered density change was the main mechanism to drive the pore-fluid flow in stage II2. (5) Through the geochemical analysis, it is believed that the mixing of magmatic hydrothermal fluid with atmospheric precipitation water and the cooling of ore-forming fluid were the main mechanisms to cause metal precipitation during Pb-Zn mineralization in the Ergu Pb-Zn deposit.

3. Computationally Simulating the Hydrothermal Ore-Forming System Involved in the Ergu Pb-Zn Deposit

3.1. The Mathematical Model for the Hydrothermal Ore-Forming System

According to the related chemical and physical laws as well as the three fundamental scientific principles in nature, namely mass conservation, energy conservation and momentum conservation, the mathematical governing equations for the hydrothermal ore-forming system under consideration are written as follows [54,55]:

\[ \frac{\partial}{\partial x}(\rho_f u) + \frac{\partial}{\partial y}(\rho_f v) = Q_f \]  

\[ u = -\frac{k(\phi)}{\mu(T)\Delta x} \frac{\partial p}{\partial x} \]  

\[ v = -\frac{k(\phi)}{\mu(T)(1 - \rho_f g)} \frac{\partial p}{\partial y} - \rho_f g \]  

\[ \rho_f c_{ref} \left( v \frac{\partial T}{\partial y} + u \frac{\partial T}{\partial x} \right) = \left( \frac{\partial}{\partial y}(\lambda^c \frac{\partial T}{\partial y}) + \frac{\partial}{\partial x}(\lambda^c \frac{\partial T}{\partial x}) \right) + QT \]  

\[ \lambda^c = \phi \lambda_f + (1 - \phi) \lambda_s, \quad \rho_f = \rho_{ref}[1 - \beta_T(T - T_{ref})] \]  

\[ \left( u \frac{\partial C_{H_2S}}{\partial x} + v \frac{\partial C_{H_2S}}{\partial y} \right) = \left( D_m \frac{\partial^2 C_{H_2S}}{\partial x^2} + D_m \frac{\partial^2 C_{H_2S}}{\partial y^2} \right) - \phi k_R C_{H_2S}C_{SO_2} \]  

\[ \left( u \frac{\partial C_{SO_2^-}}{\partial x} + v \frac{\partial C_{SO_2^-}}{\partial y} \right) = \left( D_m \frac{\partial^2 C_{SO_2^-}}{\partial x^2} + D_m \frac{\partial^2 C_{SO_2^-}}{\partial y^2} \right) + \phi k_R C_{H_2S}C_{SO_2} \]  

\[ \left( u \frac{\partial C_{H^+}}{\partial x} + v \frac{\partial C_{H^+}}{\partial y} \right) = \left( D_m \frac{\partial^2 C_{H^+}}{\partial x^2} + D_m \frac{\partial^2 C_{H^+}}{\partial y^2} \right) + 2\phi k_R C_{H_2S}C_{SO_2} \]  

where \( u \) is the \( x \)-direction component of the pore-fluid velocity with a unit of meter per second; \( v \) is the \( y \)-direction component of the pore-fluid velocity in the fluid-saturated porous rock with a unit of meter per second; \( p \) is the pore-fluid pressure with a unit of Newton per square meter; \( T \) is the porous rock temperature with a unit of Celsius degree; \( \rho_f \) is the pore-fluid density with a unit of kilogram per cubic meter; \( Q_f \) is the pore-fluid source term with a unit of kilogram per cubic meter per second; \( k(\phi) \) is the permeability of the porous rock with a unit of square meter; \( \mu(T) \) is the pore-fluid dynamic viscosity with a unit of Newton per square meter, which is dependent on temperature; \( \rho_{ref} \) is the pore-fluid reference density with a unit of kilogram per cubic meter; \( T_{ref} \) is the porous rock reference temperature with a unit of Celsius degree; \( \beta_T \) is the pore-fluid thermal volume-expansion coefficient with a unit of unity per Celsius degree; \( g \) is the gravity acceleration in the vertical direction with a unit of meter per square second; \( \lambda_f \) is
the pore-fluid thermal conductivity coefficient with a unit of Watt per meter per Celsius degree; \( c_{pf} \) is the pore-fluid specific heat with a unit of Joule per kilogram per Celsius degree; \( Q_T \) is the heat source with a unit of Watt per cubic meter; \( \lambda_s \) is the porous (dry) rock thermal conductivity coefficient with a unit of Watt per meter per Celsius degree; \( C_{H_2S} \), \( C_{SO_2^-} \), and \( C_H^+ \), are the concentrations of \( H_2S \), \( SO_2^- \) and \( H^+ \) with a unit of kilo-Mole per cubic meter in the pore fluid, respectively; and \( D_m \) is the diffusion coefficient of the solute with a unit of square meter per second.

It needs to be pointed out that from a physical point of view, Equation (1) is the mass conservation equation of the pore fluid in the considered hydrothermal system. Equations (2) and (3) are Darcy’s law, which is utilized to describe the pore-fluid flow in the fluid-saturated porous rock. Equation (4) is the energy conservation equation of the considered hydrothermal system. The first expression of Equation (5) represents the overall thermal conductivity of the fluid-saturated porous rock, while the second expression of Equation (5) represents the pore-fluid density, which is dependent on temperature. Equations (6)–(8) are the mass conservation equations of \( H_2S \), \( SO_2^- \) and \( H^+ \) in the considered hydrothermal system, respectively.

Note that in deriving the aforementioned mathematical governing equations, the following chemical reaction processes are also considered [54,55]:

\[
H_2S + 2O_2 \overset{k_R}{\iff} SO_4^{2-} + 2H^+ \tag{9}
\]

\[
Pb^{2+} + H_2S \iff PbS + 2H^+ \tag{10}
\]

\[
R = k_RC_{H_2S}C_{SO_4^{2-}} \tag{11}
\]

\[
C_{pb^{2+}}^e = \frac{C_{H^+}^2}{K_{Pb}C_{H_2S}} \tag{12}
\]

\[
MR_{Pb} = u \frac{\partial C_{pb^{2+}}^e}{\partial x} + v \frac{\partial C_{pb^{2+}}^e}{\partial y} \tag{13}
\]

where \( R \) is the experimental reaction rate of the mixing between the sulfide and sulfate fluids with a unit of kilo-Mole per cubic meter per second [56]; \( k_R \) is the overall reaction rate constant with a unit of cubic meter per kilo-Mole per second, which is strongly dependent on temperature; \( C_{pb^{2+}}^e \) is the equilibrium concentration of Pb in the pore fluid with a unit of kilo-Mole per cubic meter; \( K_{Pb} \) is the chemical equilibrium reaction constant, which is a dimensionless quantity [54,55]; \( MR_{Pb} \) is the mineralization rate of galena with a unit of kilo-Mole per cubic meter per second.

Due to the versatility of the FEM, it has been used for solving scientific and engineering problems of many different kinds [57–59]. Without exception, the FEM can be used to solve hydrothermal ore-forming problems associated with the convective flow of the pore fluid within porous rocks [54,55,59].

3.2. The Computational Models for Simulating the Hydrothermal Ore-Forming Mechanism Associated with the Ergu Pb-Zn Deposit

In the dual length-scale approach [60], two computational models for simulating the hydrothermal ore-forming mechanism associated with the Ergu Pb-Zn deposit need to be established. One computational model is called the regional model (i.e., the large length-scale model), while another can be called the deposit model (i.e., the small length-scale model). The primary advantage in using the dual length-scale approach is the fact that the overall convective pore-fluid flow pattern can be simulated in the computational simulation of the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit, while the detailed Pb distribution pattern can be simulated in the computational simulation of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. In particular, the
boundary conditions of the deposit model can be accurately and consistently determined through considering the simulating results of the regional model.

3.2.1. The Geometric Shapes and Finite Element Meshes of the Computational Models

According to the geological data and the ore-forming model of the Ergu Pb-Zn deposit [3,4], the two computational models can be established. Figure 3 shows the established two computational models. The height and length of the regional model are 10 km and 15 km. The geometry of the deposit model is an irregular polygon, which is used mainly to reduce the computational load of the numerical simulation. The maximum length and width of the deposit model are 0.6 km and 0.9 km, respectively. The purpose of setting the lateral extent of the computational domain at a large value of 15 km in the regional model is to avoid the boundary effects on the simulating results of the regional model. Particularly, the post-solidification influence of the intruded magma on the regional mineralization is primarily considered in the regional model, while the influence of the fault zone on the orebody location is primarily considered in the deposit mode. For these reasons, the solidified magma is artificially placed but not simulated in the left part of the regional model, while the fractured area of a high permeability is placed in the deposit model through considering the geological data at the corresponding location. The whole computational domains of both the regional model and the deposit model are filled with the Qianshan Formation limestone rock and the related skarn rock.

Figure 3. The geometry of the Ergu deposit: (a) the geometry of the regional model; (b) the geometry of the deposit model.
For both the regional and deposit models, Figure 4 shows their finite element meshes. In the large length-scale model, a coarse mesh of 7033 six-node triangular elements is utilized for simulating the computational domain of the regional model, while in the small length-scale model, a fine mesh of 10,078 six-node triangular elements is utilized for simulating the computational domain of the deposit model. For the purpose of ensuring the accuracy of the simulation results, the mesh Peclet number requirement is satisfied in the process of determining the maximum size of the finite element for both the regional model and the deposit model [58,61]. Consequently, the minimum side length of the finite elements used in both the regional model and the deposit model is equal to 100 m and 6 m, respectively.

![Figure 4](image)

**Figure 4.** The finite element meshes of the two computational models: (a) the finite element mesh of the regional model; (b) the finite element mesh of the deposit model.

### 3.2.2. The Parameters of the Computational Models

In computationally simulating the hydrothermal ore-forming mechanism associated with the Ergu Pb-Zn deposit, the related parameters are listed in Table 1. In order to consider the pore-fluid dynamic viscosity of the temperature-dependent feature, the following expression is used in the computational simulation [62–64]:

$$\mu(T) = 2.414 \times 10^{-5} \times 10^{(\frac{247.8}{T+133.15})}$$  

(14)
where the unit of temperature is Celsius degrees (i.e., °C). It can be observed that in the case of the pore-fluid temperature being 20 °C, the reference viscosity is equal to 10^{-3} \text{ N} \cdot \text{s/m}^2, as expected from the previous studies [65–67].

<table>
<thead>
<tr>
<th>Material Type</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pore fluid</td>
<td>Dynamic viscosity</td>
<td>Equation (14)</td>
<td>N·s/m²</td>
</tr>
<tr>
<td></td>
<td>Reference density</td>
<td>1000</td>
<td>kg/m³</td>
</tr>
<tr>
<td></td>
<td>Volumetric thermal expansion coefficient</td>
<td>2.07 × 10^{-4}</td>
<td>1/°C</td>
</tr>
<tr>
<td></td>
<td>Specific heat</td>
<td>4200</td>
<td>J/(kg × °C)</td>
</tr>
<tr>
<td></td>
<td>Thermal conductivity coefficient</td>
<td>0.6</td>
<td>W/(m × °C)</td>
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<td>Limestone</td>
<td>Porosity</td>
<td>Equation (15)</td>
<td>-</td>
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<tr>
<td></td>
<td>Permeability</td>
<td>Equation (16)</td>
<td>m²</td>
</tr>
<tr>
<td></td>
<td>Specific heat</td>
<td>2.8</td>
<td>W/(m × °C)</td>
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<tr>
<td></td>
<td>Thermal conductivity coefficient</td>
<td>850</td>
<td>J/(kg × °C)</td>
</tr>
<tr>
<td>Fracture</td>
<td>Porosity</td>
<td>0.25</td>
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</tr>
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<td></td>
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<td></td>
<td>Thermal conductivity coefficient</td>
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<td>J/(kg × °C)</td>
</tr>
</tbody>
</table>

The porous rock porosity generally depends on the burial depth, particularly at shallow depths where the mechanical compaction, diagenesis and pressure solution may modify the initial porosity during burial [68–72]. For this reason, the following expression, which states that the porosity decreases exponentially with the burial depth [73], is used for the limestone rock in this study:

\[ \phi(h) = Ae^{(-Ch)} + B \]  

(15)

where \( \phi(h) \) is the limestone rock porosity, which is a dimensionless quantity; \( h \) is the burial depth with a unit of kilometer; and \( A \) and \( B \) are two dimensionless parameters, while \( C \) is a parameter with a unit of unity per kilometer. For the limestone rock considered in this study, \( A \) and \( B \) are selected to be 0.1 and 0.05, while \( C \) is selected to be 0.75. This means that at the surface of the upper crust, where the burial depth is equal to zero, the reference porosity of the limestone rock is equal to 0.15, while the reference permeability of the limestone rock is equal to 1.0 × 10^{-15} \text{ m}^² [73].

For the purpose of considering the variation in permeability with porosity, it is necessary to select a formula to express the relationship between the permeability and porosity. In terms of dealing with this particular issue, permeability (that is a macroscopic property) depends essentially on the detailed structure of a porous medium including pore and particle shapes, pore size distributions, particle packing ways, pore connectivity and particle components. In theory, the permeability should be a function of all these factors. However, in practice, because it is very difficult, if not impossible, to quantitatively measure these factors, it is common to use porosity for approximately representing the detailed structure of a porous rock, so that the permeability is described as a function of the porosity only. Due to this approximate treatment, the porosity–permeability relationship is usually dependent on the rock type. Consequently, different porosity–permeability relationships, such as the Carman–Kozeny formula [74], the modified Fair–Hatch formula [75,76] and the Verma–Pruess formula [77] have been used to represent different rock types for simulating the dependence of permeability on porosity [78]. In particular, Nield and Bejan [79] commented that “the Carman-Kozeny law is widely used since it seems to be the best simple expression available”. Therefore, the Carman–Kozeny law is used in this study; although, the effect of using different porosity–permeability relationships deserves further investigation in future research.

Based on the above-mentioned consideration, the porosity–permeability relationship used in the computational simulation of this study can be written as
where \( k(\phi) \) is the porous rock permeability with a unit of square meter; and \( k_{\text{ref}} \) and \( \phi_{\text{ref}} \) are the reference permeability with a unit of square meter and the reference porosity, which is a dimensionless quantity, of the porous rock.

3.2.3. The Boundary Conditions for the Computational Models

For the regional model of the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit, the corresponding boundary conditions can be described as follows. Based on the annually averaged temperature of about 10 °C in the LXR, the temperature at the top boundary of the regional model is assumed to be equal to 10 °C. On the other hand, based on the regional geothermal gradient of about 30 °C/km in the LXR, the temperature at the boundary of the solidified magma and the bottom boundary of the regional model is assumed to be equal to 325 °C, because the depth of the regional model considered in this study is equal to 10 km. Except for the portion of the solidified magma, both the two lateral boundaries of the regional model are impermeable in the horizontal direction, while the solidified magma boundary is impermeable in the normal direction along the boundary. The bottom boundary of the regional model is impermeable in the vertical direction. In addition, except for the portion of the solidified magma, both the two lateral boundaries of the regional model are heat-isolative in the horizontal direction. All the porous rocks are initially saturated with water. The pore-fluid pressure at the top boundary of the regional model is equal to the atmospheric pressure (i.e., \( p_a \)). The concentration of \( H_2S \) and \( SO_4^{2-} \) are equal to zero and 0.01 kmol/m\(^3\) at the top of the regional model, while the concentration of \( H_2S \) and \( SO_4^{2-} \) are assumed to be equal to 0.001 kmol/m\(^3\) and zero at the boundary of the solidified magma in the regional model, respectively.

According to the dual length-scale approach [60], the boundary conditions of the deposit model for simulating the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit should be accurately and consistently determined through considering the simulating results of the regional model.

4. The Simulating Results of the Hydrothermal Ore-Forming System Involved in the Ergu Pb-Zn Deposit

4.1. The Simulating Results of the Regional Model

Figure 5 shows the distributions of the temperature, excess pore-fluid pressure and pore-fluid velocity in the regional model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. Since the considered hydrothermal ore-forming system is in the supercritical state, the convection of pore fluid occurs in the regional model. It is noted that in Figure 5a, the simulated geothermal gradient in the regional model is approximately equal to 30 °C/km at large, especially in the right part of the regional model. This fact indicates that the assumption of the temperature at the boundary of the solidified magma in the regional model being equal to 325 °C can be roughly justified [80]. As shown in Figure 5c, the convective flow of pore fluid is observable from the pore-fluid velocity distributions. Because of the convective flow of the pore fluid, the distribution of temperature is highly localized within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit, as can be clearly seen through observing the simulation results, which are displayed in Figure 5a. Since the temperature distribution affects the pore-fluid density distribution, as shown in Figure 5b, the abnormal distribution of excess pore-fluid pressure is capable of occurring within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. Consequently, the pore-fluid convection can be maintained in the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit.
displayed through the related simulation results. Except for $\text{SO}_4^{2-}$, which is widely distributed in the regional model (see Figure 6b), $\text{SH}_2$ and $+H$ are mainly distributed around the solidified magma (see Figure 6a and Figure 6c). This means that the convective flow of pore fluid may lead to the localized distributions of these chemical species within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. In particular, the sulfate fluid comes from the rain water on the upper crust surface, while the sulfide fluid comes from the hot magma in the deep Earth. The convective pore fluid brings $\text{SH}_2$ into the considered hydrothermal ore-forming system from the deep strata, while it brings $\text{SO}_4^{2-}$ into the considered hydrothermal ore-forming system from the shallow strata. Consequently, these two chemical species can be mixed to enable chemical reactions to occur at the appropriate place within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. More importantly, through the mixing and chemical reactions of the sulfide and sulfate fluids, the concentration gradient of $+H$ can be formed within the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit. This phenomenon is obviously observable through the simulating results shown in Figure 6c.

Figure 5. Computational simulation results of the regional model: (a) temperature (°C); (b) excess pore-fluid pressure (N/m²); (c) pore-fluid velocity (m/s).

Figure 6 shows the concentration distributions of $H_2S$, $\text{SO}_4^{2-}$ and $H^+$ in the regional model of the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit. In this figure, the localized distributions of these chemical species are obviously displayed through the related simulation results. Except for $\text{SO}_4^{2-}$, which is widely distributed in the
regional model (see Figure 6b), $H_2S$ and $H^+$ are mainly distributed around the solidified magma (see Figure 6a,c). This means that the convective flow of pore fluid may lead to the localized distributions of these chemical species within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. In particular, the sulfate fluid comes from the rain water on the upper crust surface, while the sulfide fluid comes from the hot magma in the deep Earth. The convective pore fluid brings $H_2S$ into the considered hydrothermal ore-forming system from the deep strata, while it brings $SO_4^{2-}$ into the considered hydrothermal ore-forming system from the shallow strata. Consequently, these two chemical species can be mixed to enable chemical reactions to occur at the appropriate place within the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. More importantly, through the mixing and chemical reactions of the sulfide and sulfate fluids, the concentration gradient of $H^+$ can be formed within the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit. This phenomenon is obviously observable through the simulating results shown in Figure 6c.

4.2. Determining the Boundary Conditions of the Deposit Model from the Simulating Results of the Regional Model

As stated previously, the simulating results of the regional model can be used to determine the boundary conditions of the deposit model in an accurate and consistent manner. Figure 7 shows the boundary conditions, which need to be applied to the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. In this figure, the lines identified with “Up” and “Down” are the boundary conditions, which need to be applied to the up boundary and down boundary of the deposit model, while the lines identified with “Left” and “Right” are the boundary conditions, which need to be applied to the left boundary and right boundary of the deposit model. It needs to be pointed out that since the relative location of the deposit model is clearly marked in the regional model, as shown in Figure 3, the specific locations of the above-mentioned boundaries of the deposit model can be easily found in the regional model. This means that the abscissas in the left column of Figure 7 represent the $x$ coordinates along the corresponding boundaries of the deposit model, while the abscissas in the right column of Figure 7 represent the $y$ coordinates along the corresponding boundaries of the deposit model. Because there are five fundamental unknown variables, namely the temperature, excess pore-fluid pressure, concentration of $H_2S$, concentration of $SO_4^{2-}$ and concentration of $H^+$, within the considered hydrothermal ore-forming system, it is necessary to apply boundary conditions for each of them in the deposit model of the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit. From this figure, it is clearly observed that the boundary values applied to the deposit model are no longer constants for each of the five fundamental unknown variables. In particular, without using the obtained simulating results through conducting the computational simulation of the regional model, it would not be possible to correctly determine the realistic boundary conditions, which need to be applied to the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. This fact demonstrates that the simulating results, which are the obtained numerical solutions through computationally simulating the regional model of the hydrothermal ore-forming system, play a very important role in correctly determining the boundary conditions, which need to be applied to the deposit model of the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit.
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Figure 6. Computational simulation results of the regional model: (a) concentration of \( \text{H}_2\text{S} \) (kmol/m³); (b) concentration of \( \text{SO}_4^{2-} \) (kmol/m³); (c) concentration of \( \text{H}^+ \) (kmol/m³).
Figure 7. The boundary conditions applied to the deposit model: (a) temperature (°C); (b) excess pore-fluid pressure (N/m²); (c) concentration of \( \text{H}_2\text{S} \) (kmol/m³); (d) concentration of \( \text{SO}_4^{2-} \) (kmol/m³); (e) concentration of \( \text{H}^+ \) (kmol/m³).

4.3. The Simulating Results of the Deposit Model

Figure 8 shows the distributions of the temperature, excess pore-fluid pressure and pore-fluid velocity in the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. It can be clearly observed that in the fracture zone of the deposit model, there are remarkably abnormal distributions of the temperature, excess...
pore-fluid pressure and pore-fluid velocity, especially for the excess pore-fluid pressure and pore-fluid velocity, as clearly displayed in Figure 8b,c. It is also noted that the focusing of hydrothermal fluid may occur within the fracture zone of the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. This fact indicates that more hydrothermal fluids may flow through the fracture zone in the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit.

Figure 8 shows the concentration distributions of $H_2S$, $SO_4^{2-}$ and $H^+$ in the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit.
It is noted that in the fracture zone of the deposit model, there are remarkably abnormal concentration distributions of $H_2S$, $SO_4^{2-}$, and $H^+$, especially for the concentrations of $H_2S$ and $H^+$ (see Figure 9a,c). This is mainly because the abnormal distributions of temperature and pore-fluid velocity within the fracture zone can alter the mixing and chemical reactions of these chemical species in the deposit model of the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit.

Figure 9. Computational simulation results of the deposit model: (a) concentration of $H_2S$ (kmol/m$^3$); (b) concentration of $SO_4^{2-}$ (kmol/m$^3$); (c) concentration of $H^+$ (kmol/m$^3$).
4.4. The Simulating Results of the Mineralization Rate

According to the modern mineralization theory [54,55], the mineralization rate of a specific mineral, which is expressed in Equation (13), can be used to identify the mineral precipitation and dissolution regions in the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. Theoretically, the negative value of the mineralization rate indicates the precipitation region of the specific mineral, while the positive value indicates the dissolution region of the specific mineral. Figure 10 shows the comparison of the computationally simulated Pb precipitation region with the observed Pb distribution [3] in the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit. Since the computationally simulated Pb precipitation region is identical to the observed Pb distribution [3], it may be concluded that the convective flow of the pore fluid is the primary dynamic mechanism for controlling the Pb mineralization in the hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. In addition, the good agreement of the computationally simulated Pb precipitation region with the observed Pb distribution [3] also indicates that the assumption of the \( H_2S \) concentration being 0.001 (kmol/m\(^3\)) at the boundary of the solidified magma in the regional model can be roughly justified [80]. The above-mentioned conclusion can further demonstrate that the computational simulation method associated with the emerging field of computational geosciences is a useful tool for identifying the main dynamic mechanism, which controls the mineralization pattern in the hydrothermal ore-forming system within the Earth’s upper crust.

![Figure 10. Comparison of the computationally simulated Pb distribution pattern with the observed Pb distribution: (a) the observed Pb distribution [3]; (b) the computationally simulated Pb precipitation pattern in the deposit model.](image)

5. Conclusions

Through using both the FEM and the dual length-scale approach for simulating the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit, the following primary conclusions can be made from this study: (1) the convective flow of the pore fluid can occur within the regional model (i.e., the large length-scale model), but it cannot take place within the deposit model (i.e., the small length-scale model); (2) the convective flow of the pore fluid is the primary dynamic mechanism for controlling the Pb mineralization in the hydrothermal ore-forming system involved in the Ergu Pb-Zn deposit; (3) the boundary conditions of the deposit model can be accurately and consistently determined through considering the simulating results of the regional model in a strictly scientific manner; and (4) the computational simulation method associated with the emerging field of computational geosciences is a useful tool for identifying the main dynamic mechanism, which controls the mineralization pattern in the hydrothermal ore-forming system within the Earth’s upper crust.
It should be pointed out that the work presented in this study has a limited application scope, because it is only valid for the specific situation that is established on the bases of a steady-state or a quasi-steady-state hydrothermal ore-forming system associated with the Ergu Pb-Zn deposit. Nevertheless, the effects of the transient process associated with the magma solidification and cooling on the formation of the Ergu Pb-Zn deposit may need to be considered in the future research.

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