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Acquisition of temporal-spatial geochemical information in ore-forming and carbon-dioxide sequestration systems: Computational simulation approach

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ABSTRACT

Temporal-spatial distributions of geochemical data in geoinformatics are very important for mineral exploration in the upper crust of the Earth and for the treatment of geoenvironmental issues such as CO_2 sequestration in geological formations. To understand ore-forming processes associated with mineral exploration, it is necessary to acquire geochemical information regarding orebody formation and mineralization in hydrothermal systems within the upper crust of the Earth in the past. On the contrary, to generate a safe design for CO_2 sequestration in a geological formation, it is necessary to predict the composition of geochemical environment after CO_2 sequestration and test such predictions through acquiring geochemical information in the future, so that the safety and feasibility of the design can be adequately assessed. The computational simulation approach is used, in this paper, to facilitate and guide these acquisition procedures. To demonstrate the feasibility and usefulness of the computational simulation approach in this aspect, a simplified ore-forming system associated with the Australian Broken Hill Pb and Zn mine, which belongs to a natural system, and a fluid-rock reaction system involving CO_2 sequestration in a geological formation, which belongs to a man-made system, are considered to model geochemical information. The related computational simulation results demonstrate that the computational simulation method is not only applicable for simulating the ore-forming processes in hydrothermal systems within the upper crust of the Earth, but also useful for acquiring both the ancient geochemical information associated with ore-forming systems and the future geochemical information associated with geoenvironmental systems.

1. Introduction

The temporal-spatial distribution of geochemical information in geoinformatics is very important for assessing whether or not an ore deposit is of economic value for mining. For a given geographical location, the traditional way of acquiring the geochemical information is first to obtain the related geochemical information in a point by point manner and then to generate contours of equal-value for the relevant geochemical elements at this geographical location. Obviously, this traditional way is exactly the same as what was commonly used to generate the contour of equal-elevation of a topographic map in geoinformatics. For this reason, the traditional way of acquiring the geochemical information can be called a form of geochemical mapping (Darnley, 1995; Xie and Zheng, 1983; Xie et al., 1997). Because the constituents of rock specimens are unevenly distributed in space, the geochemical data measured from a single rock specimen is usually of limited representative value in a considered volume unless this considered volume is very small. However, the geochemical data measured from the specimens of stream sediments can be used to approximately reflect the rock average constituents in a relatively larger volume. Consequently, the specimens of stream sediments were commonly used in the geochemical mapping (Darnley, 1995; Xie and Zheng, 1983; Xie et al., 1997). Nevertheless, the major limitation of using geochemical mapping is that the temporal-spatial distributions of rock constituents at depth in the Earth's crust cannot be effectively determined in detail, to say nothing of determining the controlled dynamic processes of orebody formation and mineralization in the upper crust of the Earth (Zhao et al., 2008, 2009).

From the scientific point of view, ore-forming systems within the upper crust of the Earth can be treated as complex science systems involving nonlinearly-coupled geophysical and geochemical processes between rock deformation, pore-fluid flow, heat transfer, mass transport and various types of chemical reactions (Zhao, 2015; Zhao et al., 2008, 2009, 2014). Based on this recognition, an ore deposit can be viewed as the direct consequence of synergic interactions between these geophysical and geochemical processes.

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Owing to the nonlinearly-coupled characteristics of such synergic interactions, both thermodynamic instability (Zhao et al., 2008, 2009) and chemical dissolution-front instability (Zhao, 2014) can take place in ore-forming systems. General speaking, thermodynamic instability (Zhao et al., 2008, 2009) can cause convective pore-fluid flow and therefore lead to highly localized spatial distributions (i.e. anomalies) of pore-fluid flow velocity, temperature and geochemical elements (i.e. chemical species) within the ore-forming system. Similarly, chemical dissolution-front instability (Zhao, 2014) can create highly-localized flow channels and therefore result in highly localized spatial distributions (i.e. anomalies) of pore-fluid flow velocity and geochemical elements within the ore-forming system.

From modern mineralization theory in the emerging computational geoscience (Zhao et al., 2002a, 2008), the mineralization rate (i.e. MR) of a specific mineral is directly proportional to the scalar product of pore-fluid flow velocity and the equilibrium concentration gradient of this specific mineral. Since the equilibrium concentration of a specific mineral is directly dependent on the spatial distributions of pore-fluid pressure, temperature and concentrations of other chemical species under consideration, the MR of this specific mineral is also directly proportional to the scalar product of pore-fluid flow velocity and the pore-fluid pressure gradient, temperature gradient and concentration gradients of other chemical species involved in the relevant ore-forming system. This clearly indicates that the spatial distributions of geochemical elements are also strongly dependent on the spatial distributions of pore-fluid pressure, temperature and concentrations of other chemical species involved in the ore-forming system. The main scientific reasons for this phenomenon are as follows: (1) except for the molecular diffusion of a geochemical element, pore-fluid flow can cause the advection/dispersion of geochemical elements; (2) because the chemical reaction rate of a geochemical reaction is commonly dependent on temperature, the spatial variation of temperature can cause spatial variations of the chemical reaction rate and therefore affect the spatial distribution of geochemical elements. For these reasons, the emerging computational geoscience method is very useful not only for simulating detailed ore-forming geophysical and geochemical processes within the upper crust of the Earth (Gow et al., 2002; Ord et al., 2002; Schaubs and Zhao, 2002; Sorjonen-Ward et al., 2002), but also for determining the temporal-spatial distributions of geochemical elements in geoinformatics. This can be demonstrated through two simplified examples in this study.

Keeping the above considerations in mind, the forthcoming contents of this paper are arranged as follows. In Section 2, a simple model of the Pb and Zn deposit of Broken Hill, Australia is selected to illustrate how to use the observed geochemical anomalies (that are represented by the spatial distributions of Pb and Zn ores) to reveal the spatial distributions of the main geochemical elements involved in the ore-forming process. In this case, it is necessary to consider an inverse problem, in which the spatial distributions of Pb and Zn ores are known at the present time but the spatial distributions of the main geochemical elements involved in the ore-forming system during orebody formation and mineralization in the past are unknown. Thus, the geophysical and geochemical processes involved in the ore-forming system need to be determined through several computational simulations. In Section 3, a fluid-rock reaction system involving K-feldspar alteration reaction is used to illustrate how to use the known geophysical and geochemical processes involved in a CO_2 sequestration system in a sandstone aquifer to determine the spatial distributions of the key geochemical data involved in this system in the future. In this situation, it is necessary to consider a forward modeling problem through computational simulations. However, this model is also relevant to the formation of the alteration patterns associated with the Witwatersrand gold-uranium deposit (Barnicoat et al., 1997). Finally, some conclusions drawn from this study are given in Section 4.

2. Spatial distributions of key geochemical data during lead and zinc ore-formation and mineralization associated with the Broken Hill deposit, Australia

2.1. Geological background of the Broken Hill lead and zinc deposit

The Palaeoproterozoic Broken Hill Block (Cook and Ashley, 1992) is located in central western New South Wales, Australia (see Fig. 1). It has undergone a complex deformation history during the Olarian Orogeny between 1.60 to 1.58 Ga (Page and Laing, 1992) and Delamerian Orogeny between about 520 to 490 Ma (Forbes et al., 2004; Harrison and McDougall, 1981). The Broken Hill Inlier, western New South Wales, comprises the polydeformed Early Proterozoic Willyama Supergroup, which consists of metasedimentary rocks and metavolcanic rocks deposited within an intraplate rift basin (Stevens et al., 1988) between about 1.73 to 1.64 Ga (Forbes et al., 2004; Nutman and Ehlers, 1998). The Willyama Supergroup (Stevens et al., 1988) has been divided into several major stratigraphic groups on the basis of detailed lithological mapping. The basal units of the Willyama Supergroup (Thackaringa Group and underlying packages) comprise migmatitic gneiss and quartzofeldspathic rocks intercalated with psammopelites. These rocks were deposited at about 1.71 Ga (Forbes et al., 2004; Love, 1992). Overlying these rocks is the Broken Hill Group, which is a package of pelitic to psammopelitic metasediments and minor calc-silicate rocks, amphibolites and basic gneisses. These rocks have dominantly sedimentary protolith, although numerous quartz-feldspar-biotite gneisses have been interpreted partially as deformed volcanic rocks that were deposited at 1.69 Ga (Page and Laing, 1992; Zhao et al., 2015). These are overlain by the Sundown and Paragon Groups, which is a succession of psammite, pelite, calc–silicate rocks and graphitic phyllite and schist, interpreted to have been deposited during the post-extensional evolution of the basin (Walters, 1996; Willis et al., 1983). This sequence of rocks has a maximum depositional age of about 1.64 Ga (Forbes et al., 2004; Page and Laing, 1992).

2.2. Computational simulation of the ore-forming processes associated with the Broken Hill lead and zinc deposit

The genesis of the Broken Hill Pb-Zn deposit is quite disputable. Some researchers propose that it be syngenetic, with a sedimentary origin (Haydon and McConachy, 1987; Stanton and Russell, 1959), but others propose that it be epigenetic (Rothery, 2001; White et al., 1995). The dominant mineral assemblages of the Broken Hill block result from the second event of high grade metamorphism occurred at about 1.69 Ga, although minor mineral and structural re-equilibrium occurred at the waning stages of high grade metamorphism (Plimer, 1976). An event of lower amphibolite grade retrogression occurred at about 500 Ma (Richards and Pidgeon, 1963) and these retrograde rocks are essentially restricted to transgressive shear zones.

The orebody has been metamorphosed and deformed by all of these events but if the orebody is hydrothermal in origin it is possible that mineralization occurred early in the folding history. We explore a model where mineralization occurs early in the folding history of the Broken Hill orebody, but envisage that the mineralization processes of the Broken Hill deposit can be decoupled from the major deformation processes occurred at the Broken Hill block. Thus, the mineralization problem associated with the Broken Hill deposit can be treated as a nonlinearly-coupled problem between pore-fluid flow, heat transfer, mass transport and chemical reaction processes (Zhao et al., 2008, 2009, 2014). Although the geochemical processes associated with the formation of the Broken Hill Pb and Zn deposit may involve many chemical reactions and geochemical elements, only the key geochemical reactions and geochemical elements are considered in the computational models, because they play a critical role in controlling the spatial distribution patterns of Pb and Zn ores in the Broken Hill Pb and Zn deposit (Zhao et al., 2008, 2014). On the other hand, from