An optimized potential field geological modeling method for a high-level radioactive-waste geological disposal repository

Tao Li¹, Peinan Li², Tao Zhang³, Jun Liu⁴, Xiaobin Duan³
¹ College of Civil Engineering, Tongji University, Shanghai 200092, China
² College of Environmental Science and Engineering, Donghua University, Shanghai 201602, China
³ Broadvision Engineering Consultants Co. Ltd., Yunan 650200, China
⁴ College of Urban Railway Transportation, Shanghai University of Engineering Science, Shanghai, 201602, China
* Correspondence: 2110019@tongji.edu.cn ORCID: 0000-0003-3261-4675

Abstract. A three-dimensional geological model that incorporates spatial information efficiently and intuitively is an important basis for the planning, construction, and utilization of high-level radioactive waste (HLW) disposal geological repository sites. However, traditional modeling methods cannot describe extremely complex geological contexts accurately due to the sparsity of effective data. This paper proposed a cokriging gradient interpolation method based on integrated potential fields that combines relationship and orientation data from outcrop descriptions, contour lines, boreholes, and stratigraphic contacts. A multi-stratigraphic sequence was constructed via a curve/surface tracking algorithm, and optimal geological interfaces were screened using universal cokriging equations. The geological modeling for a HLW disposal repository shows that under different data completeness conditions, this method can reveal the spatial distribution of geological structures (including fault networks and intrusive bodies), achieve better approximations for complex geological environments, and provide strong support for HLW repository roadway planning.

1. Introduction
The safe disposal of high-level radioactive waste (HLW) guarantees environmental protection and underpins the sustainable development of nuclear energy. Sealed surrounding rock can act as a natural barrier against nuclide migration [1]; therefore, geological disposal is the preferred method. As a 10,000-year project, a HLW disposal repository must maintain long-term geological and hydrological stability, have complete and solid surrounding rocks and contain no underground water sources [2]. To prevent the migration of nuclides, roadways must be specially configured to avoid possible faults and water-bearing channels. Therefore, it is necessary to construct a 3D model that incorporates spatial distributions and relationships and ascribes the characteristics of geological bodies. However, as the datasets from preliminary surveys are constructed mainly from geological mapping and few controlled boreholes, they cannot fully overcome the concealment, complexity, and uncertainty of geological conditions [3]. Traditional interpolation methods for regional geological bodies modeling based on boreholes [4] or sections will inevitably encounter the problem of low accuracy; furthermore, it is difficult to describe deep geological bodies precisely [5]. Therefore, studying geological modeling methods based on multsource constraint information and predicting the internal structural characteristics of geological bodies along with the spreading trend of geological interfaces are necessary ways of improving modeling accuracy [6]. At the same time, the combined
use of multiple data, such as fault networks, geological sections and boreholes, can construct 3D models of complex regional structures that correspond more closely to actual geological bodies [7]. The potential field method possesses superiority for integrating discrete interface points and polarized orientation data [8] and is suitable for the geological modeling of issues for which only a small volume of outcrop data are known from initial surveys. By combining multiple related variables obtained via site observations, the cokriging method can realize the prediction of geological attributes and determine weight coefficients through its semi-deviation function [9]. Therefore, this paper proposes an optimized potential field interpolation modeling method based on cokriging that combines the geological knowledge of fault networks with sequence identification to construct a 2D boundary/3D surface and a complex geological model for the Beishan preselected HLW geological disposal repository is established. Through a robustness verification, the modeling method is proven to perform well for deep geological environment predictions under conditions of low data density. This confirms its significance as a reference for repository site selection and roadway design optimization.

2. Methodology

2.1. Geological modeling method based on outcrops
Potential field interpolation is a specially designed method for constructing deep geological models based on surface outcrops; it is defined as a scalar field $T(p)$ in geological space, and by constructing a series of equipotential surfaces, the description of geological layers is achieved [10]. Geological structures, i.e., strata, are equivalent to an attribute set surrounded by two equipotential interfaces, and the value of any point on the strata is the same as the potential field. Taking a sedimentary environment as an example, the geological conditions of different spatial distributions can be distinguished by the temporal field. The controlling factor of the potential field is time distribution, i.e., the stratigraphic boundary is characterized as an isochronous surface [11]. The data for constructing a potential field $T(p)$ can be divided into two categories: 1) positioning points on the geological interface, and 2) gradient data polarized in the direction of a new formation, such as rock formations or fault orientations. There is no need for the overlap of interface points and direction points, and the gradient information can be located anywhere.

A cokriging interpolation characterizes multivariate joint spatial characteristics and predicts correlated variance based on observational data. Based on the known point set $P$ of the same geological interface, the potential field increment at point $p$ relative to the reference point $p_0$ can be estimated, as follows:

$$\Delta T(p) = \sum_{\alpha = 1}^{m} \lambda_{\alpha} (T(p_{\alpha}) - T(p_0)) + \sum_{\beta = 1}^{n} \mu_{\beta} \frac{\partial T(p_{\beta})}{\partial \beta},$$

(1)

where $p_{\alpha}, \alpha = 1, \ldots, m$ are points on the interface to which point $p$ belongs, and $p_{\beta}$ are the known gradient data points of the geological interface. $\lambda_{\alpha}$ and $\mu_{\beta}$ are the coefficients that determine the interpolation weight. Function 1 can be solved under a cokriging framework by minimizing the estimated variance. $T(p)$ is assumed as a spatial random function with polynomial drift and a stationary covariance, and the drift form is shown in Function 2:

$$m(p) = \sum_{l=0}^{L} b_{l} f_{l}(p),$$

(2)

where $m(p)$ is the polynomial drift, $f_{l}(p)$ is the $l$th order sub-term at point $p$, and $b_{l}$ is the corresponding coefficient term.

2.2. Complex geological interface interpretation based on surface tracking technology
Compared with the conventional kriging system, the main challenge of the potential field interpolation algorithm based on geostatistical cokriging is how to reasonably construct the potential field $T(p)$ and the covariance function $K(.)$ using a small volume of data [12]. Although $K(.)$ can be preliminarily constructed by assuming an a priori covariance model, usually, the experience-based a priori covariance model introduces larger errors. After completing the preliminary geological modeling, the
real effective and reasonable verification comes from the covariance function after analyzing and fitting the actual sampled data. Aiming to avoid the difficulty and subjective arbitrariness of the covariance function of the potential field and the cross-covariance, this paper proposes an optimized potential field interpolation algorithm. The core framework steps of the geological potential field tracking algorithm are described briefly, as follows:

(1) Construct a geological scalar function/potential field $T(\rho)$ and conduct a complex geological interface interpolation; since the interpolation does not introduce dimensionality reduction effects, the tracking and simulation of extremely distorted and irregular geological interfaces are more convenient.

(2) Interpolate the background vector field based on the geostatistical cokriging method. Using the directional information in geological sampling, uniformly distributed polarization unit vectors are cokriged on the background grid; since the direction information and its covariance function are easier to obtain, a better interpolation result can be achieved.

(3) Generate a geological geometric interface using the curve/surface tracking algorithm. Taking sequence recognition, borehole, or stratigraphic contact information as a strong constraint (or pass) condition, the 2D geological boundary/3D surface trajectory is generated using the curve/surface tracking algorithm, and finally, multiple locally optimal curves/surface paths are generated with optimization and adjustment using directional data.

(4) Determine the final geological stratification interface/line: In the case of multiple (or locally optimal) alternative paths, by comparing and analyzing errors, this paper uses cokriging equations (Function 1) to filter out an optimal search trajectory surface/line as the spatial geometric expression of the stratum interface/line under the weighting constraint of $\mathbf{T}(\rho) - \mathbf{T}(\rho') = 0$.

3. Multisource data-processing method

3.1. Definition of fault–grid relationship
A fault can correspond to a special type of stratum; but a series of discrete points cannot reveal the boundary and deep direction of a large-range fault. To simplify the considerations, faults are assumed to be extensions to the boundary of a modeling area when there is no truncation boundary, and a fault
is represented by an equipotential surface through the modeling area. However, under normal circumstances, faults in different periods behave as network topology structures that intercept or dock with each other; this docking relationship can be determined by relying on multi-point survey data.

3.2. Sequence and contact relationship recognition

The geological interface model of a single potential field is represented as infinitely extending equipotential surfaces. The isosurfaces cannot intersect. However, a real geological body behaves in a crossover-type relationship (e.g., cutting, overwriting, or intrusion) under the action of sedimentation or erosion. A complete description of a geological environment requires the integration of multi-potential fields, and the relationship between such fields is determined by the stratigraphic sequence (temporal) and the contact (spatial). In this paper, the sedimentary order of the strata is identified by the sequence recognition result obtained by geophysical [13] and geochemical [14] technologies. The stratigraphic contact relationship defines the spatial topological relationship of the strata, including its conformity, parallel/angular unconformity, erosion, deposition, and faults. Conformity and parallel unconformity are modeled according to multiple approximately parallel isosurfaces. The boundary conditions of the potential field are defined mainly by the two contact relations of erosion and onlap, and each layer model is established according to the sequence. Therefore, two basic stratigraphic contact relationships are defined for potential field modeling: 1) The erosion contact relationship allows any stratigraphic sequence to appear and cuts off older stratigraphic sequences, and 2) onlap contact makes no fundamental changes or differences in the geometry of a certain stratigraphic sequence compared with older stratigraphic geometry.

4. Case study

4.1. Beishan site condition

Beishan is located in the Jiuquan area of Gansu Province and is characterized by scarce precipitation, high evaporation, complete rock masses, and low-permeability surrounding rock; therefore, it is the preferred area for China’s HLW geological disposal repository. This section provides a 3D geological description and a model reconstruction for the Jiujing section of the Beishan area. The Jiujing section has a hilly terrain, and its structural deformations are mainly fractures and fissures followed by ductile shear deformation. This belt is part of the tectonic magma belt at the northern margin of the Tarim Plate. Mesoproterozoic and Neoproterozoic magmatism is extremely active here, and granite-like geological bodies comprise the crystalline base of the study area.

![Figure 3. Geological map of the Beishan area](image-url)
4.2. Outcrop data

A major advantage of the potential field interpretation method is that it can predict the overall spatial trend of deep rock masses and establish a preliminary regional geological structure model by integrating surface orientation and contact data without using borehole and profile information. Due to the lack of drilling data, to further understand the large-scale stratigraphic distribution, the deep geo-environment, and the fault-cutting network of the repository, a 1:50,000 regional survey and an environmental assessment were re-launched, and a total of 357 observation points of longitude, latitude, altitude, contact surface, and rock formation data were obtained, as shown in Figure 5. The average inclination angle of each measurement point was 52° to 64° in the ESS direction. The inclination angles of all faults in the study area were almost 70°, which belongs to the deep-cut layer. These 2D observational data are used mainly for constraining deep geological geometrical structures or the volumes of intrusive granite rocks to support preliminary modeling.

The sequence relationship pattern in the study area is shown in Table 1.

| Strata name | Contact | Color | Lithology | Cutting fault |
|-------------|---------|-------|-----------|---------------|
| DQSS        | Onlap   | AnChDdk^2 | Dolomite quartz schist | F2–F6, F12, F14 |
| QS          | Onlap   | AnChDhy^1 | Quartzite section | F6 |
| PSS         | Onlap   | AnChDhy^2 | Phyllite schist section | F2–F6 |
| ASS         | Onlap   | AnChDhy^3 | Amphibolite schist section | F1–F3, F6 |
| MS_1        | Onlap   | AnChDdk^3 | Quartz marble section, quartz schist | F11 |
| UHASS       | Onlap   | AnChDhyj^3 | Upper-high alumina schist section | F1 |
| MMG         | Erode   | P_Sηγ | Muscovite monzonitic granite | F1, F6 |
4.3. Geological Modeling of high-level waste disposal repository

Since the repository relies mainly on an intrusive granite rock series with a stable geological environment and robust mechanical properties, this paper conducts a reconstruction of a 3D model for a HLW disposal repository by integrating the direction and contact data from the preliminary regional survey; this includes an outcrop description, a field direction measurement, and a cross-sectional interpretation map. This paper focuses mainly on the structural characteristics of extensive intrusive volcanic rocks and the distribution of metamorphic and sedimentary rock series. The model’s size is 28 × 17 × 2 km.

Table 1 processes the stratigraphic sequence, fault network, stratigraphic contact, and outcrop data according to Chapter 3. The changes in the thickness of different strata are not related, the spatial variability is complex, and the partial singularity of the stratigraphic exposure traces is very severe; therefore, first, a digital elevation model is established using a topographic map. Then, the potential field model of each formation is interpolated independently based on outcrop data, i.e., a preliminary
geological model is generated. Finally, multiple potential fields are integrated, and the model shown in Figure 6 is optimized according to Section 2.2. This paper’s work is realized based on the GeoModeller software package [15]. The model shows that the intrusive rock series belonging to the Jiujing unit (Pt²J65β) covers the widest range, while the thickest intrusive rock series is the porphyritic monzonitic granite of the Bantan unit (Pt²B1y). In the southern part of the study area, the sedimentary and metamorphic rock sequences show large dips and tend to face away from the intrusive rock series, and stratigraphic inversion occurs in some areas (Figure 6).

4.4. Robustness analysis of the optimized potential field interpolation method

A stable geological barrier is a final defense against radionuclide migration to the natural environment, and a repository requires the long-term stability of a wide range of hydrological and geological environments; in particular, the high-permeability fault zone should be avoided. To evaluate the stability of the potential field interpolation method in low data density conditions, this paper randomly removes positioning point and contact data according to the ratio shown in Figure 8 and generates five comparison models.

The geological model in Figure 7b accurately includes the overall geological structural characteristics of the research area, but deviations are inevitable in some regions. When the input data decrease to 50%, Figure 8d shows that there is still a high correlation with the original field observations. When the volume of data drops to 30% (Figure 8e), although the boundaries become continuously smooth as the data density decreases, there is still a good correspondence between the model and the outcrop distribution in the geological map. The results indicate that the new interpolation method is effective for 3D geological structural modeling, and it can also represent the overall geological shape and structural characteristics even in areas of low data density. Therefore, this method is suitable for geological modeling when the original data density or quantity cannot be guaranteed. By eliminating local irregularities caused by inferior data, the accuracy of the model is assured.

![Figure 8. Robustness analysis of geological modeling: (a) modeling result of the original data volume; (b-f) modeling results of different data reduction](image)

5. Conclusion and discussion

Due to the lack of deep underground data for the Beishan HLW disposal repository, this paper proposed an optimized potential field cokriging modeling algorithm. The algorithm was used to establish a complex geological model for the repository in GeoModeller that realizes the prediction and approximation of complex geological bodies. The results show that it is possible to construct a regional model based on limited available outcrop and constraint data; the model not only demonstrates the geological structural characteristics and stratigraphic fault relationships of the study area but also clearly shows the following: (1) how the surface information controls the geometry of the deep strata/fault system, (2) how to express the overlying and intrusive contact relationship between rock layers, and (3) the degree of influence between the fault network and the stratigraphic sequence. The model can be verified and optimized with future detailed survey data (e.g., spatial...
directions/gradients from deep boreholes and seismic explorations) to achieve a high degree of accuracy. However, the potential field interpolation effect depends on whether a fine cokriging semi-deviation function can be constructed, which depends on the quality and distribution of the data. Moreover, the algorithm tends to be spatially smooth, leading to weaknesses in dealing with problems of spatial disproportion, such as pinching and unexposed strata, which can be further solved using the uncertainty method or by manual adjustment. Additionally, a series of works can be carried out based on the established model, including the overall site evaluation of the repository, the design optimization of roadways by the introduction of a roadway structural model, the evaluation of roadways and surrounding rocks, and the spatial prediction of surrounding rock levels. All of these will provide strong reference points for the site selection, design, and construction of a repository.

ACKNOWLEDGEMENTS
This research work was instructed by Peinan Li and was funded by the Science and Technology Innovation and Demonstration Project of the Department of Transport of Yunnan Province ([2019] No. 36).

References
[1] Wang, J., Progress of Geological Disposal of High-level radioactive waste in China in the 21st century. Atomic Energy Science and Technology, 2019. 53(10): p. 2072–2082.
[2] Swift, P.N. and E.J. Bonano, Geological disposal of nuclear waste in tuff: Yucca Mountain (USA). Elements, 2016. 12(4): p. 263–268.
[3] Shu-cai, L., et al., State of Art and Trends of Advanced Geological Prediction in Tunnel Construction. Chinese Journal of Rock Mechanics and Engineering, 2014. 33(v.33;No.283): p. 1090–1113.
[4] Bing-yin, T., et al., A fast progressive 3D geological modeling method based on borehole data. Rock and Soil Mechanics, 2015. 36(12): p. 3633–3638.
[5] Guangjun, J., et al., Accuracy factors of 3D geological modeling and quality control. Journal of Guilin University of Technology, 2020. 40(01): p. 85–94.
[6] Howell, J.A., A.W. Martinius, and T.R. Good, The application of outcrop analogues in geological modelling: a review, present status and future outlook. Geological Society, London, Special Publications, 2014. 387(1): p. 1–25.
[7] Jørgensen, F., et al., Combining 3D geological modelling techniques to address variations in geology, data type and density–An example from Southern Denmark. Computers & Geosciences, 2015. 81: p. 53–63.
[8] Chao-dong, F., Y. Peng, and X. Bo, Rapid geological modeling by using implicit 3D potential field interpolation method. 2010 International Conference on Computer Design and Applications, ICCDA 2010, 2010. 5.
[9] Chang-hong, W., Z. He-hua, and Q. Qi-hu, Application of Kriging methods and multi-fractal theory to estimate of geotechnical parameters spatial distribution. Rock and Soil Mechanics, 2014. 35(Supp2): p. 386–392.
[10] Calcagno, P., et al., Geological modelling from field data and geological knowledge. Physics of the Earth and Planetary Interiors, 2008. 171(1–4): p. 147–157.
[11] Chiles, J.-P. Modelling the geometry of geological units and its uncertainty in 3D from structural data: the potential field method. 2004. Citeseer.
[12] Che, D. and Q. Jia, Three-Dimensional Geological Modeling of Coal Seams Using Weighted Kriging Method and Multi-Source Data. IEEE Access, 2019. 7: p. 118037–118045.
[13] Ye, Y., et al., Application of element geochemistry in the identification of sequence stratigraphy. Journal of China Coal Society, 2014. 39(S1): p. 204–211.
[14] Zhaojun, L., et al., Distinguishing features and their genetic interpretation of stratigraphic sequences in continental deep water setting: A case from Qingshankou Formation in Songliao Basin. Earth Science Frontiers, 2011. 18(4): p. 171–180.
[15] Geophysics, I., GeoModeller. intrepid-geophysics. com. 2015.