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Coupled modeling between geological structure fields and property parameter fields in 3D engineering geological space

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ABSTRACT

3D geological modeling is becoming ubiquitous in the visualization and analysis of the subsurface geological characterization that involves both geometrical structure and various properties. The engineering geological space consists of two types of data fields: one is the geological structure field and the other is the property parameter field. There are two kinds of relationships, i.e. superposition and coupling, between property parameter fields and geological structure fields. While many of the current modeling techniques have proven to be quite useful for modeling and visualization of geological structures or property parameters independently, they were never designed for the purpose of handling the coupling relationship among different data fields. This shortcoming seriously limits the reliability and practicality of the computer models, and there is a pressing need to build a meaningful 3D spatial model that involves both geometry and properties. In this paper, we present a novel modeling framework for the coupled modeling and analysis of geo-objects in 3D engineering geological space. There are three innovative improvements in this framework. First, a mixed 3D spatial data model, which is a combination of boundary representation and Geocellular, is designed to address the need for the unified description of geometry and topology of geo-objects as well as their internal properties. And then, in order to obtain geologically reasonable property models controlled by geological constraints, the qualitative geological constraints are converted into quantitative control parameters in data preprocessing stage, and different property interpolation schemes are used respectively to handle different types of geo-objects. And finally, in order to gradually refine 3D geological models, the iterative modeling technique is imported, and an efficient mechanism for information feedback and error correction is set up. This coupled modeling framework is well-suited to produce detailed 3D geological models attributed with physical, chemical, engineering or hydrogeological parameters, and intuitively analyze property characteristics within each modeled unit and their spatial relationships in 3D.

1. Introduction

During the construction process of large and complex engineering structures in urban areas, there is increasing demand to obtain a precise definition of subsurface conditions in engineering geological space. Therefore, it is necessary to completely depict geological structural features and spatial variations of property parameters (including physical, chemical, engineering and hydrogeological features) within individual geological objects (Hack et al., 2006; Turner, 2006; De Rienzo et al., 2008; Royse et al., 2009; Font-Capó et al., 2011). The traditional methods for representing engineering geological information, whether using two-dimensional paper maps/reports or digitized CAD drawings, became insufficient as they are difficult to meet the requirements of the actual applications (Hack et al., 2006; Turner, 2006; Royse et al., 2009). Nowadays, several sophisticated technologies, such as geographic information system (GIS), spatial database, computer graphics and 3D visualization, have been used by geologists and engineers to build solid models of geological objects in 3D. 3D geological models not only can express the temporal and spatial distributions of geotechnical units and spatial variations of property values with an intuitive and vivid way, but also can be used to express, verify and modify geological

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cognition/judgment/knowledge built up by geologists. Based on 3D models, it is convenient to present geo-objects, which previously potentially existed in the minds of geologists, to planners, engineers, developers, policy-makers and the general public, and to perform quantitative spatial analysis and professional applications.

3D geological models, especially those which are based on geological concepts, can be widely used to gain insight into the subsurface. Engineers, geologists and developers can use the models to visualize and analyze relationships between structural features and property characteristics within specific geological units. The huge interests and needs drawn from the planning and development of engineering geological space drive the development of 3D geological modeling and visualization. In the past 20 years, 3D modeling in engineering geological space has attracted a great deal of attention in both geosciences and engineering fields (Jones, 1988; Jones, 1989; Culshaw, 2005; Turner, 2006; Royse et al., 2009). With joint efforts contributed by geologists, computer experts and GIS researchers, a series of sophisticated 3D modeling and analysis techniques have been developed to address the needs of subsurface structural characteristics (Mallet, 2002; Lemon and Jones, 2003; Culshaw, 2005; Turner, 2006). Numerous experiments (Dawson and Baise, 2004; Balfe et al., 2005; Turner, 2006; Royse et al., 2009; Aldiss et al, 2012; Travelletti and Malet, 2012) have indicated that 3D geological models have huge potential and added values in the reconstruction, analysis, representation and process simulation for geo-objects in engineering geological space. However, with the development of utilization for the subsurface, the much higher demand is brought up for the modeling and analysis of engineering geological bodies. The existing modeling approaches, which only built structurally simple models of geo-objects, were unable to meet the requirement of practical applications. Geotechnical engineers not only need the precise definition of the geometric shapes for the subsurface geo-objects, but also need the proper description of such property features as physical, chemical, engineering and hydrogeological properties heterogeneously distributed within geological bodies. More importantly, it will be better to couple all these subsurface characteristics into a meaningful 3D spatial model to carry out various forms of quantitative spatial analysis and professional applications. Therefore, it is an essential task to build the coupled model of geological structures and property features in 3D engineering geological space.

In this paper, we explore novel modeling techniques and associated implementation methods for building the coupled model in 3D engineering geological space, taking into account both superposition and coupling relationships between geological structures and property parameters. The rest of the paper is organized as follows. Classifications of geological data fields and 3D geological models are introduced in Section 2, which also summarizes the critical problems that modelers may encounter when trying to use the existing modeling techniques. In order to build meaningful 3D geological models attributed with property data, we present a novel modeling framework for coupled modeling between geological structure fields and property parameter fields in 3D engineering geological space. We discuss the details of the proposed modeling framework in two sections: Section 3 considers the overall framework including the modeling process and the key steps, while Section 4 concentrates on the major technical issues and some innovative improvements. In Section 5, we demonstrate an application of the coupled modeling framework to build 3D solid models in Shanghai's construction projects. Finally, the conclusions of this paper are provided in Section 6.

2. Coupled modeling in 3D engineering geological space

Computer modeling and visualization of engineering geological objects in 3D are complex processes to carry out such operations as reconstruction, representation and analysis of material, information and characterization existing in the engineering geological space. There are two different types of data fields in geological space: property parameter fields and geological structure fields. The property parameter fields, which spatially reflect the geological property characteristics (such as physical, chemical, hydrogeological or geotechnical properties within different geological bodies and the composition of individual geological bodies, as well as their control interfaces), continuously distribute in 3D space with ambiguous boundaries. The geological structure fields, which spatially reflect the geometrical shapes between the different defined geological bodies/interfaces and their compositions, have relatively clear boundaries that can be identified with additional discrete control sampled data.

In 3D geological space, property parameter fields are not only ideally coincident with geological structure fields in spatial position, but also correlated with geological structure fields in geological genesis and characteristics. Therefore, there are two kinds of relationships, i.e. superposition and coupling, between property parameter fields and geological structure fields. In engineering practice, geotechnical engineers typically determine the boundaries of the control interfaces in geological structure fields according to the distributions of the geological property characterization. But to look at it another way, the distributions of property parameter fields are also associated with the geometrical forms and buried depths of geo-objects, as well as the relative disparity between different geo-objects. The geological structure fields not only represent the spatial distribution patterns of geological bodies, but also control the spatial variation of the property parameters within individual geological units. As a consequence, engineers and geologists should also be able to deduce and predict the spatial variation of the property characterization within the site being modeled in the light of the geological structure fields, and this requirement is daily-happened in practical applications. In engineering geological space, it is essential to identify the coupling relationship between geological structure fields and property parameter fields to guide the practical modeling process during 3D geological modeling and visualization.

In 3D space, we can build geological structure models to reflect geological structure fields, and construct geological property models to interpret property parameter fields. A 3D geological structure model is a mathematical model that concentrates on the representation of spatial positions, geometrical shapes and topological relationships of geo-objects. In 3D geological structure models, property parameters within individual geological units are generally assumed to be uniform, unchanged and homogeneous (Kessler et al., 2008; Royse et al., 2009). Therefore, it is either hard or impossible to describe the spatial variability and statistical laws of the property characteristics within geological bodies (Hobbs et al., 2002). On the contrary, the 3D geological property model, which is a mathematical model attributed with geological property values for each modeled unit, is convenient to depict the heterogeneity and natural variability of property characteristics within individual geological bodies (Dawson and Baise, 2004; Balfe et al., 2005). However, it is limited by its defect in the structural description as it contains neither geometrical nor topological information. Although the 3D geological property model is suited to perform statistical calculation and comprehensive analysis, it is not appropriate in cases where geometrical shapes and topological relationships of geo-objects are required, such as statistical evaluations of geotechnical properties associated with selected formations (Hobbs et al., 2002).

Considering the above-mentioned coupling relationship between geological structure fields and property parameter fields in engineering geological space, the procedure of 3D modeling and visualization for geo-objects should be able to reflect the following workflow generally applied in the practical working process: From sampled data of property parameters → determining boundaries between different defined geological units → predicting spatial distribution of property parameters within individual geological units → verifying, generalizing and application. However, the existing 3D geological modeling processes/techniques have distinct shortcomings in implementing the above-mentioned procedure. Four critical problems that modelers may encounter when trying to use the existing modeling techniques are listed as follows.

Firstly, in the realm of 3D spatial data model, modelers are faced with the problem of lacking conventional mixed data models that are specifically suitable for engineering geo-objects. Current 3D spatial data models used to abstract, classify, describe and express geo-objects can be divided into four different categories as volumetric models, vector models, mixed models and integrated models, and there are several representational models for each subcategory (Jones, 1989; Wu, 2004). 3D volumetric data models, which are based on the spatial partition, represent a spatial object as a combination of primitive volumes (De Floriani and Falcidieno, 1988; Wu, 2004). The conventional 3D volumetric data models include constructive solid geometry (CSG), 3D-raster, octree, tetrahedral network (TEN), tri-prism (TP), generalized tri-prism (GTP), Geocellular, etc (Turner, 2006; Turner and Gable, 2007). 3D vector data models, which describe solid volumes in terms of their enclosing surfaces, emphasize on the surface representation for the spatial objects (De Floriani and Falcidieno, 1988; Wu, 2004). The conventional 3D vector data models include boundary representation (BRep), wire framework and non-uniform rational B-splines (NURBS). 3D mixed data models use two or more vector/volumetric data models to describe one geo-object at the same time. The conventional 3D mixed data models include BRep–CSG, GTP–TEN and BRep–GTP–TEN. 3D integrated data models firstly apply various single data models to describe different types of spatial objects respectively, and then integrated them into a unified 3D space to fully represent multiple types of spatial objects. The conventional 3D integrated data models include CSG + TIN + GTP, BRep + TIN + GTP and object-oriented data model. For practicality, each type of spatial data models has its advantages and disadvantages in several aspects like geometric representation, space partition, topological description and consistency maintenance. At the present time, due to the difference in their adaptabilities, the existing 3D spatial data models have more or less defects when they are used to subdivide the engineering geological space, as well as abstract, classify, describe and express geo-objects as data (Wu, 2004). Therefore, they are not appropriate in cases when a unified real-3D modeling of geological structure characteristics and property parameters within geological units is required. It is necessary to develop a vector/raster coexisted data model and associated data structure to efficiently represent all or most of engineering geo-objects.

Secondly, for the modeling procedure, the past research has typically employed “independent modeling” or “sequential modeling” process to reconstruct geological structure fields and property parameter fields individually. During the independent modeling process, geological structure fields and property parameter fields are treated as two standalone data fields. Therefore, 3D geological models, including structure models and property models, are reconstructed respectively without considering any relationship between those data fields. In the light of the superposition relationship between geological structure fields and property parameter fields, the sequential modeling process first builds a 3D structure model to reflect geological structure fields, and then subdivides the geological space into a series of 3D volumetric meshes by applying discretization methods, and finally creates a 3D property model by attaching geological property values to corresponding mesh units (voxels) (Wu and Xu, 2004). No matter independent modeling or sequential modeling procedures, the coupling relationship in geological genesis and characteristics between geological structure fields and property parameter fields is not taken into consideration. Therefore, the existing modeling procedures have serious limitations as the modeling results frequently differ from the actual subsurface conditions.

Thirdly, in the realm of the reconstruction techniques for 3D geological models, the existing methods for building 3D geological models can be divided into two categories: one is the structure modeling approach used to build 3D geometric models of geological bodies, and the other is the property modeling approach used to reconstruct 3D property parameters within geological bodies. The past research has focused on generating 3D structure models that reflect geometries and topologies of geo-objects. Over the past two decades, a series of sophisticated 3D modeling techniques have been developed to build 3D structure models from different types of data like boreholes, cross-sections and geological maps (Mallet, 2002; Wu, 2004; Wu and Xu, 2004; Wu et al., 2005; Xu et al., 2011; Travelletti and Malet, 2012; Zhang and Lei, 2013). For example, the transition probability/Markov approach was developed to simulate the spatial distribution of geologic units and facies (Carle and Fogg, 1996; Carle and Fogg, 1997; Carle et al., 1998), and its implementation program, termed TPROGS (Carle, 1999), has been incorporated into several groundwater modeling packages to model stratigraphic distributions in sedimentary environments (Weissmann and Fogg, 1999; Weissmann et al., 1999; Fleckenstein et al., 2006; Quinn, 2009). In addition, Lemon and Jones (2003) presented the horizon method for generating 3D solid models of geologic structures from borehole data, and Zhu et al. (2012) presented the Borehole–Surface–Solid method to construct discontinuous surfaces in sedimentary stratigraphic systems. However, up to now there are still fewer researches concentrating on the reconstruction of 3D property models. At present, 3D property models are typically constructed by applying automatic interpolation algorithms or geostatistics methods (like various forms of Kriging interpolation) (Deutsch and Journel, 1997; Dawson and Baise, 2004; Emery, 2004; Juang et al., 2004; Balfe et al., 2005; Baise et al., 2006). These methods are complex and inconvenient to be used to create 3D property models as they cannot consider the coupling relationship between property parameters and the complex geometries of geo-objects. Up to now, there are still no perfect methods or easy-to-handle software toolkits for the reflection of the intrinsic property heterogeneity and anisotropy of subsurface features.

Fourthly and finally, in the realm of the visualization and spatial analysis, the current techniques generally fall short of advanced functions in 3D visualization and spatial analysis for subsurface features. For the lack of the perfect 3D geospatial analysis tools, it is either hard or impossible to visualize and analyze the spatial and temporal relationships/correlations between geological structures and property parameters. And then, it is difficult to perform quantitative 3D spatial analysis on the solid models of geo-objects that contain both geometry and property features.

A true 3D solid model should not only be able to represent various kinds of subsurface information like spatial positions, geometries, topologies and properties of geologic bodies, but also has ability of 3D spatial analysis and geospatial prediction. Therefore, it should be created in the light of the coupling relationship between geological structure fields and property parameter fields, rather than separate one data field from another. A reasonable 3D geological modeling process should treat all sub-stages of modeling procedure (such as processing geological data, generating geological frameworks, reconstructing property parameter fields, 3D visualization and spatial analysis) as a unified and integrated whole. It should not only consider the indicated significance for geological frameworks in property parameter data, but also take into account the restriction effect of geological frameworks on property parameter fields. Only in this way can we achieve the final goal to build a high quality, geologically reasonable, reliable 3D geological model attributed with property data in an intuitive way.

In recent years, a large number of geologists and engineers have launched a series of exploratory researches on the coupling of 3D geological models and numerical simulation (Blessent et al., 2009; Xu et al., 2011). In this coupling, three steps are generally followed: first, 3D structure models, which represent geometries of geological bodies, are created by applying 3D geological modeling techniques; and then, different kinds of 3D mesh division models, which are attributed with abundant property information, are automatically generated from the 3D structure models; and finally, the 3D mesh models are imported into numerical simulation programs. Nowadays, two kinds of coupling patterns, data coupling and function coupling, have been developed in the coupling of 3D geological modeling and numerical simulation. Through those coupling patterns, we can successfully solve such intractable problems as difficult to build 3D geological models and divide space units in pre-processing of numerical simulation analysis for geotechnical engineering.

However, coupled modeling between geological structure fields and property parameter fields has distinct meanings and features different from the coupling of 3D geological models and numerical simulation. Some research teams have invested considerable effort on how to construct meaningful 3D geological models attributed with property data. For example, to meet the growing demand for geo-environmental information in the Thames Gateway Development Zone (TGDZ, about 1800 km^2), east of London, UK, Royse et al. (2009) have used proprietary software GSI3D (Culshaw, 2005) to create detailed 3D spatial models attributed with physical, chemical or hydrogeological parameters in TGDZ. However, due to the limitation of the modeling software and the implementation techniques, the TGDZ study only provided a single uniform property attribution to individual geological units. That is, geological properties within per layers are kept constant and only provide an average value for each modeled formation. Therefore, the modeling results may not reflect the intrinsic property heterogeneity and anisotropy of most subsurface property parameters within a modeled geological unit. Although this simplified approach is very effective for regional ground investigations in large study areas to express relationships between geologic bodies and properties from macroscopic view, it is not suited for small-and-medium-sized sites in which a more specialized analysis needs to be performed to provide a detailed understanding of natural variability of the complicated geo-objects. Patel and McMechan (2003) investigated the interpolations and extrapolations constrained by control horizons, and presented an algorithm to build gridded 2D physical property models from well log data and control horizons. But this algorithm only applied to 2D property modeling rather than 3D modeling. Zhu (2005) proposed an approach to consider the constraining effect of stratum surfaces when interpolating borehole sample data onto the 3D structured meshes. However, this approach fails to convert qualitative geological constraints into modeling rules that can be identified and programmed by computers. During the modeling process, the qualitative geological constraints, such as spatial distribution characteristics of sedimentary environment and sedimentary facies, and the interpretation and deduction from geologists, are particularly important as they also control the spatial distribution of property parameter fields.

Although the above-mentioned advances have meant that the advantages and the added values of using coupled models of subsurface geo-objects are greater, the current modeling techniques still fall short of systematic modeling theories and standard workflow for constructing coupled 3D geological models. This limitation restricts the use of 3D geological models in areas where complex coupling relationships between geological structure fields and property parameter fields must be first taken into consideration. In order to produce geologically reasonable coupled models, we must carry out deeply theoretical analysis and systematically empirical study focusing on the coupled modeling between diverse data fields in 3D engineering geological space.

3. General framework of coupled modeling in 3D engineering geological space

3.1. Modeling process

For generating 3D geological models attributed with property data, the central technical core contains the development of a simple but practical modeling framework supporting coupled modeling of geological structure fields and property parameter fields, including both structural model creation and property modeling, as well as geological data processing, 3D visualization and spatial analysis. Based on the recent developments and applications of 3D geological modeling and visualization, we present a novel modeling framework to support coupled modeling geological characterization in 3D space. This modeling framework not only comprehensively considers the superposition relationship between geological structure fields and property parameter fields, but also effectively handles the coupling relationship among diverse geological data fields. The modeling process for this coupled modeling framework is shown in Fig. 1.

3.2. Key steps

The implementation of the above-mentioned coupled modeling framework can be decomposed into nine key steps, and step-by-step execution of the modeling framework is explained below.

Step 1: *Collect geological data and convert them into a geospatial database*. The main work of the first step contains collecting geological data of the site being modeled, preprocessing raw data acquired from various sources, converting these data sets into conventional data formats suitable for 3D geological modeling, and storing them into a unified geospatial database with a universal 3D coordinate system. Geological data involves a variety of data types with different qualities, including boreholes, cross-sections, geologic and terrain maps, remote sensing data, geophysical and geochemical data, and real-time observed sample data (Chang and Park, 2004; Wu and Xu, 2004). In the data processing stage, the conventional digitization of boreholes and cross-sections can be performed by using existing software systems like AutoCAD and ArcGIS. Other operations on geo-objects, such as the identification, interpretation, comparison, description and location for geo-objects (like strata, lenses, intrusions and other complicated geological structures), should be carried out manually. More importantly, in order to ensure the accuracy of geometric shapes and keep the consistency of spatial relationships among complicated geo-objects, various qualitative geological constraints, including spatial distribution characteristics of sedimentary environment and sedimentary facies, and the interpretation and deduction from geologists, need to be converted into quantitative control parameters by means of the quantitative surface description. These quantitative control parameters are represented as a series of geological interfaces. Therefore, they can be imported into the geospatial database through a general-purposed data conversion interface (Wu and Xu, 2004; Wu et al., 2005).

Step 2: *Create an initial geological framework model by applying geometry modeling methods*. The geological framework model is a geometrically accurate representation of the fundamental geological framework, suitable for visualization by computer graphics (Turner, 2006). Since the geological framework is composed of geological surfaces, it can be organized by the boundary representation (BRep) scheme. BRep is a popular 3D vector data model that defines geo-objects by a collection of individual surrounding surfaces (De Floriani and Falcidieno, 1988). With spatial geometry data stored in the geospatial database, several often-used 3D geometry modeling methods, such as the spatial interpolation, the surface modeling, the section modeling and the interactive modeling, can be used to generate the initial geometric surfaces of geo-objects. Taking these geometric surfaces as enclosing boundaries, we can establish an initial geological framework model by the topological relationship between two adjoining surfaces.

Step 3: *Subdivide the geological framework model into volumetric meshes*. Based on well voxelized criteria for continuous geological surfaces (Cohen-Or and Kaufman, 1995), the engineering geological space can be subdivided into a series of 3D volumetric meshes by

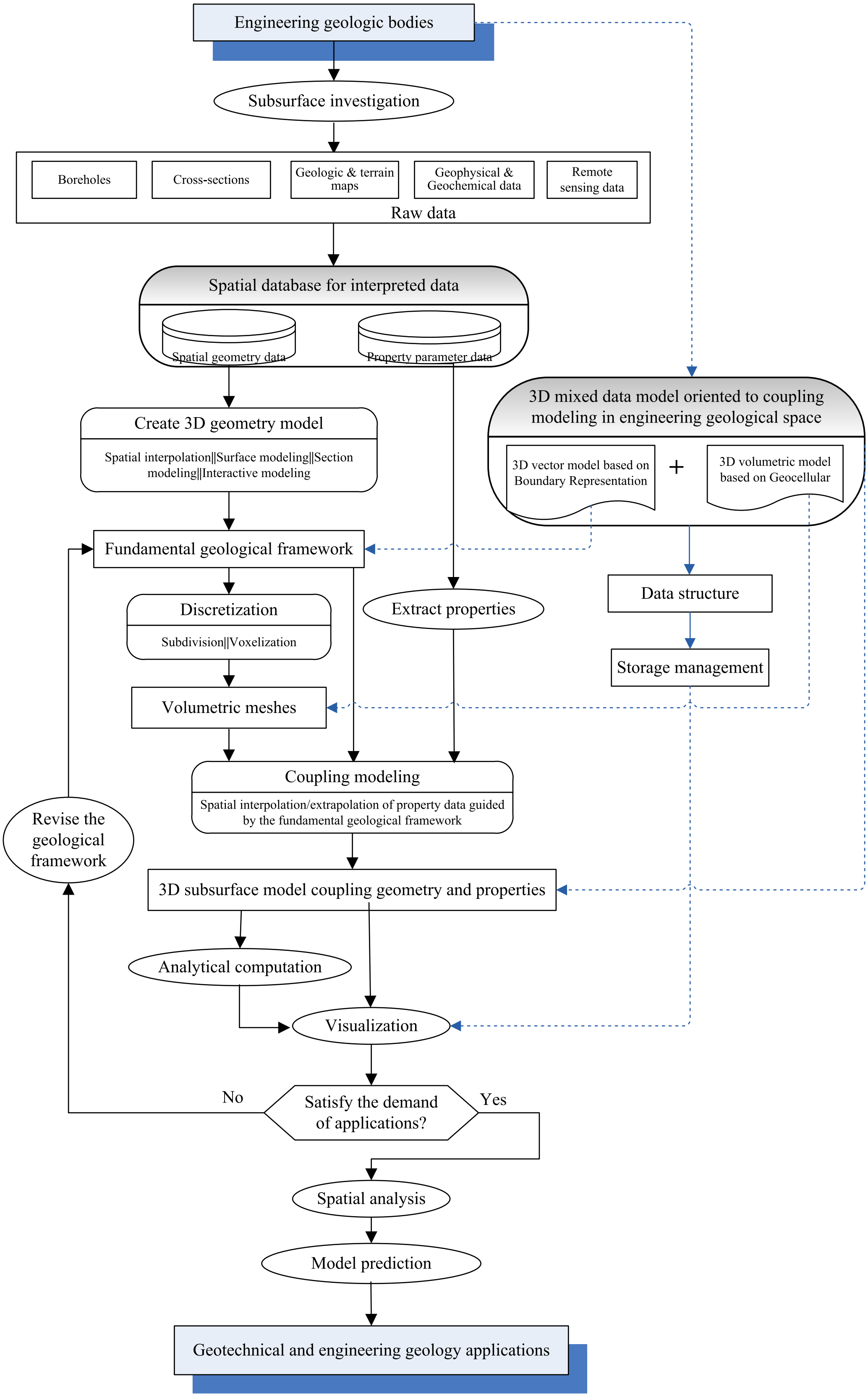


Fig. 1. The modeling process for coupled modeling in 3D engineering geological space.

applying discretization methods. Taking the fundamental geological framework as spatial reference, 3D volume solids, which consist of large numbers of partly deformable Geocellular meshes (Jones, 1988; Swanson, 1989; Denver and Phillips, 1990), can be automatically generated. Mesh sizes of Geocellular vary considerably depending on the type of geological property to be modeled, the density and detail of the data available for the modeling, as well as the available computer hardware. Typical cell dimensions in Geocellular meshes are about 0.5–2.5 m thick and 10 × 10 m areally. A typical geocellular model may have hundreds of thousands to millions of cells in it, while typical geological modeling systems can handle on the order of 10^5–10^6 simulation cells. However, large numbers of Geocellular meshes (over 10^5–10^6 cells) may create to build fine property models. In order to avoid potential clustering of cells, the total amount of Geocellular meshes should be adjusted appropriately according to the available physical memory of the computer.

Step 4: *Build 3D property model coupled with geological framework model*. In the fourth step of the modeling process, we adopt appropriate interpolation schemes to calculate geological property values attached to each Geocellular mesh, and finally create a coupled 3D geological model, which not only contains geometric structures but also attributed with geological property data. Since the fundamental geological framework controls the spatial distribution and propagation of property parameters within different defined geo-objects, geometrical guides, which are predefined by the geological framework model, should be taken into account when interpolating geological property values from known sample locations to entire 3D volumes. Due to the great differences of stratigraphic settings and structural characteristics among various kinds of geo-objects, we need to apply different interpolation schemes to deal with different types of geo-objects. More specifically, for geo-objects which have indistinct directivity and cannot be separated into layers (such as most of the metamorphic/magmatic rock strata), geostatistics methods (like various forms of Kriging) (Deutsch and Journel, 1997) can be used to interpolate property values within individual modeled unit; while for geo-objects which have distinct directivity (such as most sedimentary formations and a small number of metamorphic/magmatic rock strata), we must firstly split each modeled layer into a series of “isochronous strata” by applying particular stratified rules (Jones, 1988), and then calculate property values within each isochronous stratum by using inverse distance weighted method or linear interpolation method. After interpolation, we can produce geologically reasonable property models to reflect 3D spatial variation of geological properties within property parameter fields.

Step 5: *Display and evaluate the coupled 3D model*. The coupled model can be directly, or after processing additional analytical computation like numerical simulation (Turner, 2006), fed to a 3D visualization view for real-time visualization and analysis. Due to the coupled model which contains both geometries and properties, geometrical shapes of geo-objects and property parameters within each geological unit can be displayed and compared at the same view. We can easily detect and analyze the spatial relationships and correlations between geological structure fields and property parameter fields. In this step, we can check whether the coupled model meets the requirements of the practical applications. If the coupled model satisfies the demand of applications, just go to Step 7 to perform subsequent 3D spatial analysis; otherwise, we must go to the next step (Step 6) to revise the geological framework model and the property model.

Step 6: *Revise the framework model and property model by applying iterative method*. Once the coupled 3D geological model is in need of revision, we first carry out local refinement and adjustment to the geological framework model by utilizing error correction methods for 3D geological structure models (Zhu and Zhuang, 2010), and then go to Step 3 to redo such work as discretization of engineering geological space, construction of property model, 3D visualization and reliability assessment for the revised model. Based on this stepwise iterative method, we can gradually and effectively refine the coupled 3D geological model to a desired accuracy, and a reliable coupled 3D model that meets the requirements of the practical applications can be produced.

Step 7: *3D spatial analysis*. Using spatial analysis techniques widely applied in 3D GIS, such as distance analysis, orientation analysis, trend surface analysis, spatial correlation analysis, isoline/isosurface/isovolume analysis and spatial statistics analysis (Wu and Xu, 2004), geological structures that quantitatively control the spatial distribution of the property parameter fields can be extracted and plotted to display the variations of geological properties. In addition, quantitative spatial correlations between geological structure fields and property parameter fields can be obtained and displayed with an appealing, intuitive and easily understandable way.

Step 8: *Model prediction and verification*. Based on the quantitative spatial correlations between geometry and properties, the coupled geological model can be extrapolated to the neighboring areas of the modeling site. We can verify the prediction results with the actual underground projects (Aldiss et al, 2012), and test the practical effects of different modeling methods, especially different spatial interpolation schemes.

Step 9: *Geotechnical and engineering geology application*. The coupled 3D geological model can be used to describe, understand, predict and demonstrate the spatial relationships and correlations between geological structure fields and property parameter fields in 3D engineering geological space. We can apply the coupled model to the subsurface projects in the modeling site, conduct a comprehensive analysis and comparison, and extend the model to other sites to increase the added value of 3D geological modeling and visualization.

4. Key issues and main improvements

Compared with the existing implementations of 3D geological modeling and visualization, the major issues and associated innovative improvements for the above-mentioned coupled modeling framework involve three essential aspects: 3D spatial data model, reconstruction method for property parameter fields, and generating mechanism for coupled geological models. The following subsections are explanations of these issues.

4.1. 3D spatial data model

Since geometry, topology and property of geo-objects need to be described and analyzed coherently, a mixed data model is urgently required to express geo-objects in 3D engineering geological space. The 3D mixed data model uses two or more vector/volumetric data models to model, describe and express one geo-object at the same time. It not only inherits superiority of vector data model for fast visualization, but also takes advantage of volumetric data model for efficient spatial analysis. Thus, it well adapts to different modeling requirements derived from both various geological settings and spatial resolutions (Wu, 2004). In this paper, we design a mixed 3D spatial data model to address the need for the unified description of geometry and topology in geo-objects as well as their internal properties.

The proposed 3D mixed data model is produced by combining boundary representation (BRep) with Geocellular. BRep was originally designed for computer-aided design and manufacture in mechanical engineering. It employs hierarchical data structure to divide spatial objects into a combination of several primitive elements like vertices, edges, loops, faces, volumes, shells and regions. Due to its prominent advantages such as simple in algorithm and fast in speed, BRep is the most mature and unambiguous representation of 3D solid objects in current CAD/CAM systems. But on the other hand, BRep is complicated to maintain its data structure and topology because it describes all features of an object at the same level (De Floriani and Falcidieno, 1988). As a mutant of 3D-raster structure, Geocellular has a normal grid partition in the lateral direction (XY plane), while the spatial partition along the vertical direction (Z) is not invariable but changed according to the actual data fields or the controlling interface of geo-objects (Jones, 1988; Swanson, 1989; Denver and Phillips, 1990; Wu, 2004; Turner, 2006). Using Geocellular structure, we can produce reasonable 3D subdivisions closer to actual geological interfaces.

The implementation of the proposed 3D mixed data model is decomposed into three steps. Firstly, to describe the structural characterization in 3D engineering geological space, we employ BRep to organize the geometrical information of the geological framework model. And then, in order to express internal properties, the 3D geological space is subdivided into a series of Geocellular meshes constrained by geometric surfaces of geo-objects. And finally, to keep seamless and coherent between geometrical boundaries and Geocellular meshes, several suitable links, typically triangulated or gridded surfaces, are adopted to record and connect the same interfaces between geological frameworks and volumetric meshes. A sample application of the proposed 3D mixed data model is shown in Fig. 2.

The benefits of the proposed 3D mixed data model are obvious: it keeps conciseness and accuracy inherited from 3D vector data models, with the advantages of simplicity and universality inherited from 3D volumetric data models. Furthermore, it has a wide applicability in true 3D representation and spatial analysis as it supports predictive modeling in 3D. Therefore, it is a practical 3D spatial data model to support coupled modeling, integrated exhibition and visual analysis in 3D engineering geological space. Using this data model, we can successfully create arbitrary fine 3D meshes to model actual spatial distributions of property parameter fields by adaptively subdividing the engineering geological space.

4.2. Reconstruction method for property parameter fields

At the property modeling stage, two essential problems need to be solved to reflect the intrinsic heterogeneity of geological properties within individual geological units.

One problem is how to quantitatively express the qualitative geological constraints. Geological constraints can be classified as “quantitative” or “qualitative” constraints. A “quantitative” geological constraint is one that can be expressed by exact numerical values, such as the spatial distribution of simple stratum surfaces, and control interfaces of some particular geological bodies like faults, folds, lenses and intrusions. In contrast, other geological constraints (such as the spatial distribution characteristics of sedimentary environment and sedimentary facies, and the interpretation and deduction from geologists), which are hard to be depicted accurately, can be classified as “qualitative” geological constraints. Quantitative geological constraints are convenient to participate in the property modeling process, while qualitative geological constraints are difficult to be used directly to control the spatial distribution of geological properties. In order to quantitatively express the qualitative geological constraints, we interpret and deduce qualitative geological constraints as early as data preprocessing stage, and convert them into quantitative control parameters by means of the quantitative surface description. After that, spatial interpolations/extrapolations between sampled property data points, guiding by the quantitative geological interfaces, can be carried out. Although this method may increase the workload of data preprocessing, it is practical and easy to implement during the modeling process.

A second problem is the property interpolation within individual modeled units. Since there are significant differences in occurrence patterns among various types of geo-objects, we need to use different property interpolation schemes to handle different types of geo-objects respectively. For most of sedimentary formations, deposits (or strata) with the same geologic time usually have similar or identical geological properties. Therefore, each part of a given sedimentary stratum can be assumed as comparable, and we can carry out property interpolation within individual geological units under guidance of the concept of “isochronous stratum” (Jones, 1988). An isochronous stratum can be treated as a subordinate stratum segment. It is disassembled from the higher level stratum based on the vertical distribution character and structural relationship of the stratum. It is gradually formed during depositing process and reflects the accumulative changes of the external environment. The interface of the isochronous stratum is regarded as the contact surface between two adjacent small isochronous strata. At the property modeling stage, each sedimentary stratum can be divided into a series of isochronous strata. Because geological properties within the same isochronous stratum are highly correlated, inverse distance weighted interpolation or linear interpolation can be used to calculate property values within each isochronous stratum. In addition, when interpolating unknown property value at a given Geocellular location, only known samples from the same isochronous stratum are utilized. This method is straightforward, and also suited to some metamorphic/magmatic rock strata which have distinct directivity. For most of the metamorphic/magmatic rock strata, they have indistinct directivity and cannot be separated into layers. In this situation, geostatistics methods, typically various forms of Kriging (Deutsch and Journel, 1997), can be used to calculate property values within individual geological units. By constructing various forms of variogram function, Kriging method can easily calculate internal property values, overcome instability generated from other often-used deterministic interpolation schemes (such as inverse distance weighted interpolation, trend surface fitting interpolation and spline surface interpolation), and also provide probabilistic estimates of the uncertainty of the prediction. Moreover, each Geocellular mesh is defined by 8 cell corners and

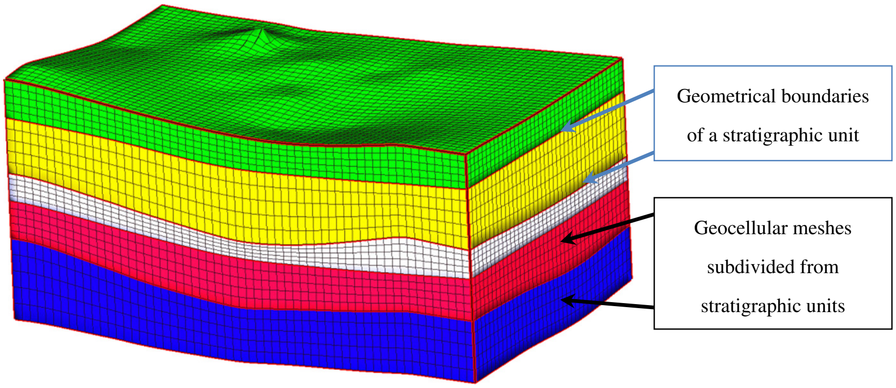


Fig. 2. A sample solid model of 3D geo-objects expressed by the mixed data model (BRep + Geocellular).

may contain one or more property parameter values. To interpolate the property value within a Geocellular mesh, we first calculate property values located in cell corners by employing deterministic or geostatistical interpolation methods, then assign the average value of the given 8 cell corners to the modeled Geocellular. During the interpolation process, the center-point clustering algorithm (Wu et al., 2005) is introduced to avoid any potential clustering of being interpolated points and known sample points. Therefore, a Geocellular mesh only gets a single value for each property parameter.

4.3. Generating mechanism for coupled geological models

3D geological models can be regarded as the consequence of a series of continuous interactions between complicated geological data and ambiguous modeling rules. Therefore, the reconstruction process of the coupled geological models must be a stepwise refinement process by performing continuous iteration and revision. During the modeling process, we can import the iterative modeling technique, and establish an information feedback and error correction mechanism to gradually and effectively refine 3D geological models.

4.3.1. Iterative modeling

For previous modeling methods, no matter they adopt independent modeling or sequential modeling procedure, the modeling process was split into two independent phases like geometry modeling and property modeling. In our coupled modeling framework, we apply the iterative modeling technique to avoid limitations that occurred from the traditional modeling procedures. The iterative modeling is based on the following five steps: (1) create a geological framework model, which consists of a variety of geological interfaces, by applying geometry modeling methods; (2) subdivide the geological framework model into a series of 3D volumetric meshes by applying discretization methods; (3) interpolate property values attached to each volumetric mesh, and create an initial coupled geological model. When interpolating geological property values from known sample locations to entire 3D volumes, geometrical guides predefined by the geological framework model should be considered; (4) locally refine and adjust the geological framework model by selecting suitable geometry modeling methods and control parameters, as well as expert knowledge/judgment/interpretation for given geological structures and their properties; and (5) go to step 2 to redo such works as described in steps 2–4 until a reliable coupled geological model is generated.

4.3.2. Information feedback and error correction

In order to produce geologically reasonable 3D models, we set up an efficient mechanism for feeding back information and correcting errors. During the modeling process, we can inspect 3D geological models on the computer screen with automatic or semi-automatic operations. Various errors, such as observation error, calculation error, interpretation error and vision error (Wu and Xu, 2004), are fed back to modelers and instantly displayed on the screen. In 3D scene, five possible methods can be used to check up errors in 3D geological models: the comparative inspection method based on geological data collected from various sources, the automatic quality inspection method based on 3D topological relationships, the logical inspection method based on property query, the manual inspection based on human vision, and the manual inspection based on 3D spatial measurement. Furthermore, we also provide some practical approaches to modify raw data, revise intermediate models or adjust their control parameters. When correcting errors in 3D geological models, there are three often-used methods: (1) optimize modeling methods, such as employing higher degree interpolation methods, utilizing particular geological laws or constraints (Zhu et al., 2012), etc.; (2) supplement or modify geological data, such as increasing additional samples, virtual boreholes or cross-sections to represent local variation of geological information (Zhu and Zhuang, 2010); and (3) revise intermediate models by applying 3D model renewal techniques (Zhu and Zhuang, 2010).

During the modeling process, we first evaluate whether the accuracy of the 3D geological models meets the requirements of the practical applications, depending on the spatial distribution of geological structures and their internal properties displayed in 3D scene; then navigate to locations where the accuracy is lower, and analyze causes of bad accuracy; and next revise 3D models by applying above-mentioned error correction methods; and finally, re-evaluate revised models, and repeat above works until the accuracy of the 3D geological models meets the requirements. We can generate interactive, modifiable, assessable and applicable 3D models by synthetically using methods described above.

5. A case study

We have implemented the proposed modeling framework in Microsoft Visual C^{++} (VC++) and the OpenGL Graphics Library (OpenGL) on the Windows platform. VC++ is an integrated, visual development environment (IDE) that enables object-oriented development of rich and highly interactive scientific application programs for the Windows platform. OpenGL, which also is widely used in scientific visualization and information visualization, is a cross-language, multi-platform application programming interface (API) for rendering 2D and 3D computer graphics. VC++ and OpenGL have been widely embraced by scientific users as a means to develop various types of application programs in one seamless interface. Without having to develop more sophisticated visualization environments from the low level, rendering and displaying of 3D models can be easily implemented by using VC++ and OpenGL toolkits. Compared with other choices (such as VB, Java and Javascript), VC++ and OpenGL have more advanced component and extension options, and the performance of this combination is the best. Therefore, in this study VC++ and OpenGL are selected for implementing the proposed modeling framework. To test the usefulness of the coupled modeling method in sites with complex relationships between geological structure fields and property parameter fields, a sample application of building 3D solid models is given below.

The study area is located on the riverside of the Suzhou River in Shanghai Putuo District, China, and covers 600 × 400 m^2. As Fig. 3 shows, there are 24 shallow boreholes detecting 5 stratigraphic units: miscellaneous fill, mucky soil, clay, silty sand and sandy silt. The strata are denoted as S_1, S_2, S_3, S_4 and S_5 from the top to the bottom. The study area is a potentially brownfield site contaminated with perchloroethylene (PCE), a common soil contaminant that is classified as a Group 2A carcinogen by the International Agency for Research on Cancer. In order to evaluate pollution of PCE in the study area, 99 subsurface soil samples are collected from boreholes, and the concentrations of PCE within all soil samples are determined in the laboratory. As illustrated in Fig. 3, the soil samples are represented as spheres, and each sphere is colored according to the PCE data value at that point.

To predict the spatial distribution of stratigraphic units and the concentration of PCE, we adopt the following four steps to reconstruct geological structure fields and property parameter fields in the study area:

Step 1: According to the boreholes obtained from the study area, a simple 3D stratigraphic model (as shown in Figure 4A) is constructed by applying the Borehole–Surface–Solid method (Zhu et al., 2012). This model describes the arrangement of the stratigraphic units in the subsurface with their real positions and full extents.

Step 2: A voxel-based solid model, which is filled with Geocellular meshes, is established by applying 3D discretization methods. As shown in Fig. 4B, the geological space is divided into 60,000 small Geocellular meshes. Mesh sizes of Geocellular are about 0.5–2.5 m thick and 10 × 10 m in the areal direction.

Step 3: Based on the fundamental geological framework predefined by the 3D stratigraphic model and a detailed analysis of the soil sample data, three contrasting 3D property models, as shown in Fig. 5A, B and C,

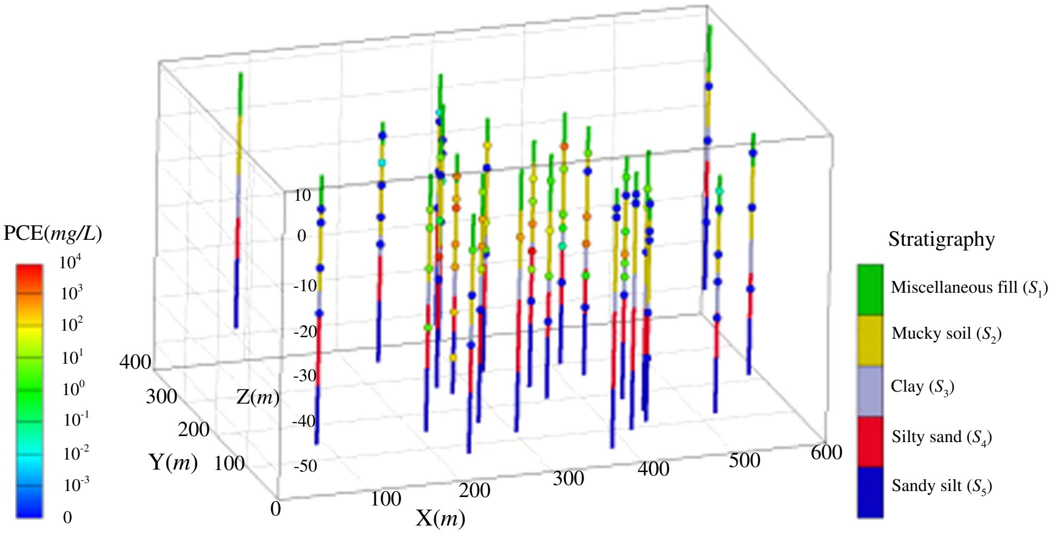


Fig. 3. Locations of boreholes with stratigraphic units (represented as colored segmental tubes), and soil samples with PCE data values located along boreholes (represented as colored spheres). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

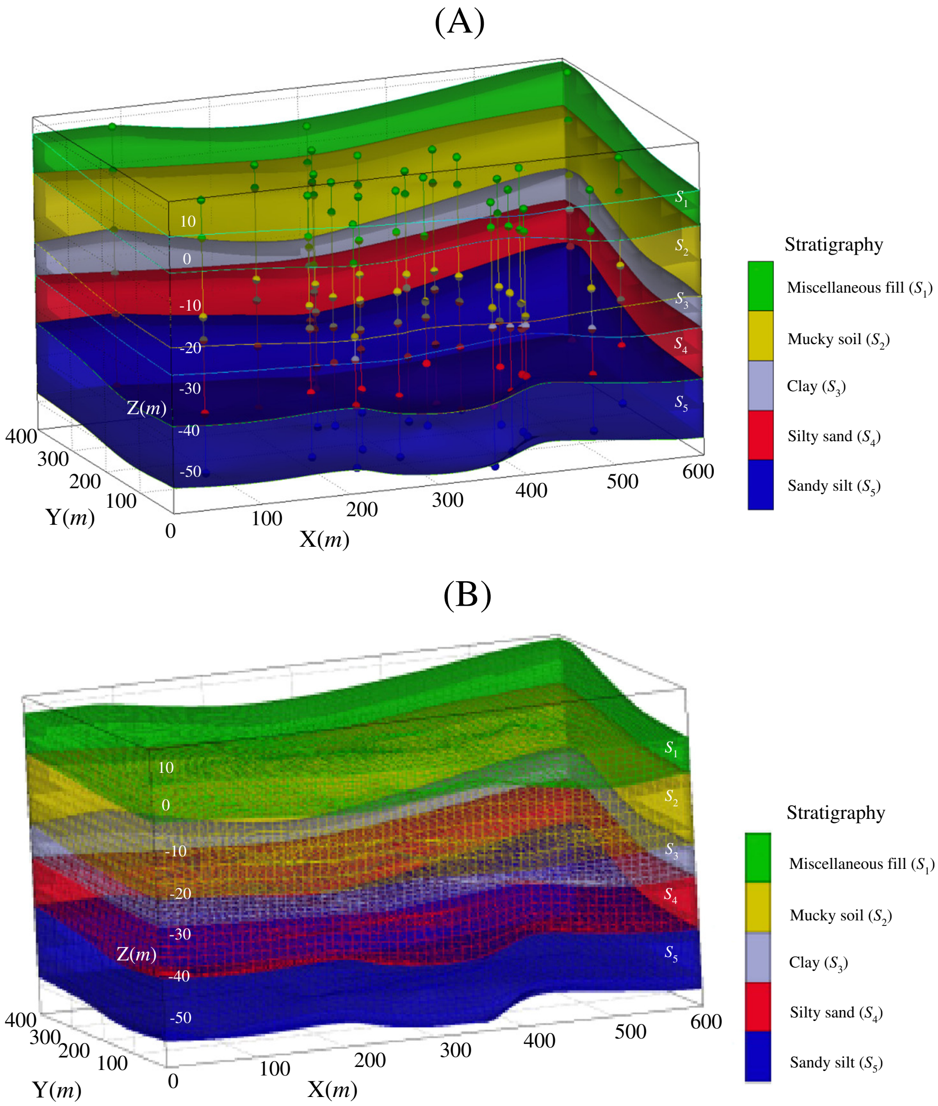
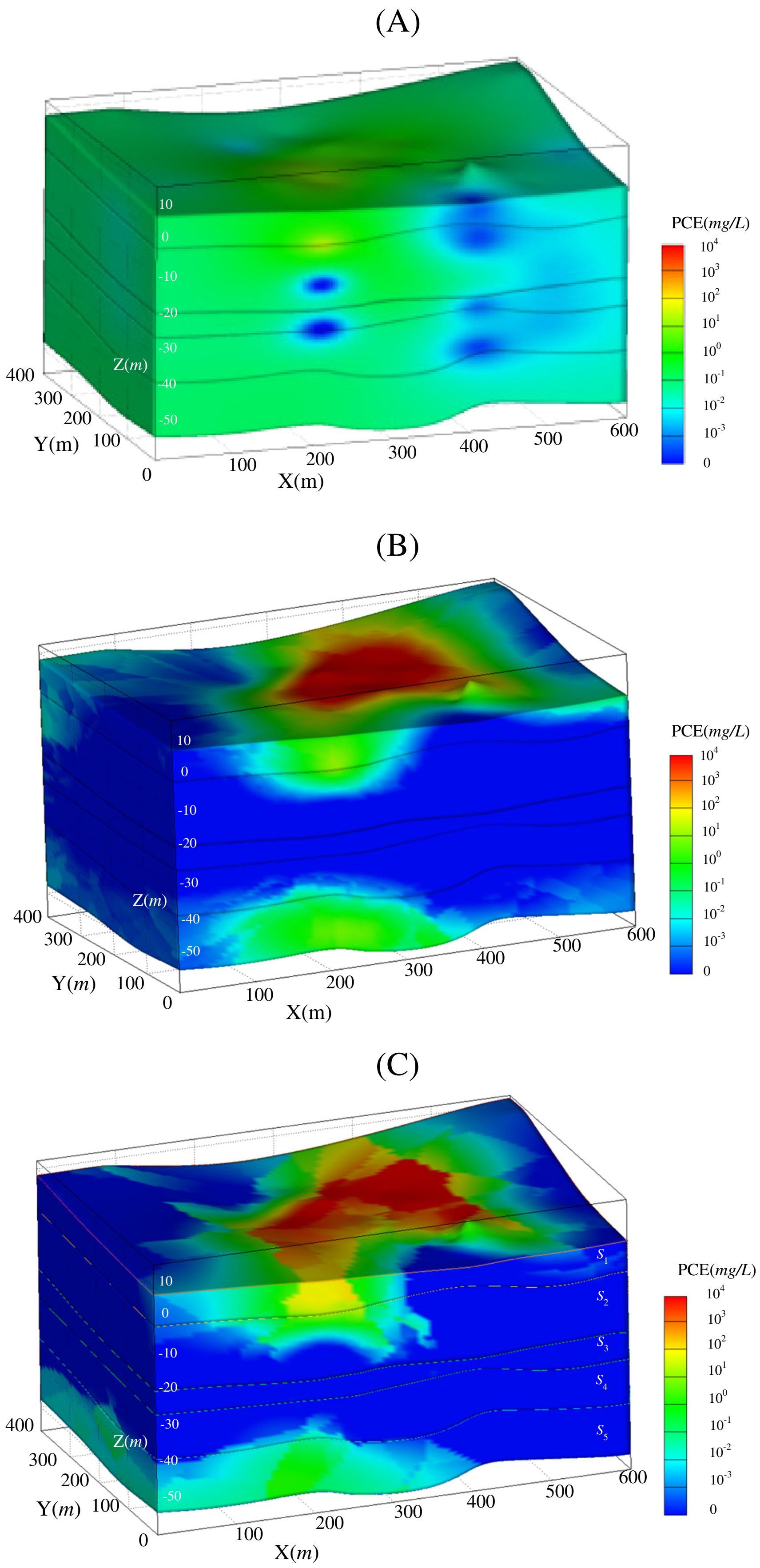


Fig. 4. 3D stratigraphic model of the study area (Transparency = 50%): (A) 3D solid model with boreholes, (B) 3D solid model filled with Geocellular meshes.


(A)
PCE(mg/L)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
0
Z(m)
10
0
-10
-20
-30
-40
-50
Y(m)
400
300
200
100
0
X(m)
100
200
300
400
500
600
(B)
PCE(mg/L)
Z(m)
Y(m)
X(m)
(C)
PCE(mg/L)
S1
S2
S3
S4
S5
Z(m)
Y(m)
X(m)

are constructed using three different interpolation schemes. In model Fig. 5A, the PCE concentration values attached to each Geocellular voxel are directly calculated using the inverse distance weighted (IDW) interpolation in the entire 3D space, without considering any structural constraint. In model Fig. 5B, we utilize the Ordinary Kriging method to interpolate PCE concentration values without thinking about the structural constraint. In model Fig. 5C, the same interpolation method as used in model Fig. 5A, IDW interpolation, is also chosen for the interpolation of PCE concentration values onto a 3D Geocellular voxel. However, the interpolation process is guided by the shape of the control strata that are predefined by 3D stratigraphic model. That is, the models Fig. 5A and B involve contributions from all samples, while the model Fig. 5C only uses sample data from the same stratigraphic unit.

Step 4: We investigate the differences between the three resulting property models and compare the selected modeling methods. By comparing the models, the tremendous differences in values and extents of the PCE concentration can be easily detected, despite similar trends for the spatial distribution of PCE in both models. In order to quantitatively evaluate the accuracy of these models, an additional borehole and 8 soil samples obtained from this borehole are compared with the solid models. The comparison result shows that the model Fig. 5C shows much higher levels of confidence in the PCE property prediction, compared to models Fig. 5A and B. This result is in line with our expectations. Therefore, we can say that the model Fig. 5C, which considers the property heterogeneity within each modeled unit, has a higher accuracy and can be used for predictive modeling. Engineers and geologists can use the model Figs. 4A and 5C to model, visualize and analyze subsurface features in the study area.

The resultant coupled 3D model (Figure 5C) can then be used to view not only the spatial distribution of stratigraphic units, but also the vertical and lateral variations in the concentration of PCE. Engineers and geologists can use the model to assist in the recognition, identification, estimation and remediation of soil pollution by PCE. At present, remediation technologies for soils polluted by PCE can be categorized into ex-situ and in-situ methods. Ex-situ methods involve excavation or extraction of polluted soils, as well as subsequent above-ground treatment or disposal (such as hauling the contaminated soil to a regulated landfill). In-situ methods, mainly including chemical treatment and bioremediation, seek to treat the contamination without removing the soils. No matter applying ex-situ or in-situ methods, the coupled 3D model can be used to provide information on the extent, depth and variability of the concentration of PCE, to help design more appropriate treatments of the contaminated soil. For example, if we use ex-situ methods, we can precisely define boundaries and depths of the excavated soils by using the coupled 3D model. If we use in-situ methods, we can use the 3D model to locate sites where contaminations are likely to occur, and hence use the most efficient chemical treatment or bioremediation, ultimately achieve the goal of decreasing the cost of the environmental remediation as well as controlling the secondary pollution.

6. Conclusions and future work

Geological modeling and visualization in 3D originated from the mineral and petroleum exploration industries. Over the past two decades, a series of dedicated computer programs have been developed to address associated technical problems. The mineral exploration industry focused on spatial modeling of geology and ore bodies, while the petroleum exploration industry concentrated on modeling property parameters within oil/gas reservoirs (Hack et al., 2006). With the increasing need of subsurface characteristics, modeling the subsurface becomes more and more important in engineering geological and geotechnical studies. Compared with the mineral and petroleum exploration industries, there are more particular requirements for 3D modeling and visualization in engineering geological space. Geotechnical engineers need to model and predict not only the geometric shapes and property features of the subsurface geo-objects, but also the spatial and temporal relationships/correlations between geological structures and property parameters. However, for the lack of a perfect mechanism to handle the coupling relationship between geological structure fields and property parameter fields, it is either hard or impossible to construct meaningful 3D spatial models of the shallow subsurface in engineering geological space only utilizing the existing modeling techniques. Coupled modeling between geological structure fields and property parameter fields is not only a stepwise process to extract subsurface information with the integration of multiple data fields, but also a continuous developing process from geo-objects to geospatial data, to geospatial information, and even to decision-making based on geological knowledge. The existing modeling techniques, no matter adopting independent modeling or sequential modeling procedure, lack systematic modeling theories and standard workflow for constructing coupled 3D geological models.

In this paper, we have developed and illustrated the general framework and associated implementation methods for building coupled models of geological structure fields and property parameter fields in 3D engineering geological space. There are three innovative improvements in this framework: (1) to address the need for the unified description of geometry and topology of geo-objects as well as their internal properties, a mixed 3D spatial data model, which is a combination of boundary representation and Geocellular, is designed; (2) to interpolate geologically reasonable property models controlled by geological constraints, the qualitative geological constraints are converted into quantitative control parameters in data preprocessing stage, and different property interpolation schemes are used respectively to handle different types of geo-objects; (3) to gradually refine 3D geological models, the iterative modeling technique is imported, and an efficient mechanism for information feedback and error correction is set up. During the modeling process, the proposed modeling framework tries to take account of both the superposition relationship and the coupling relationship between geological structure fields and property parameter fields. It overcomes limitations of the previous 3D modeling techniques which omit the coupling relationship of geological genesis and characteristics among different data fields. The most significant feature of this framework is that it has ability to encapsulate the natural variability of geological features by incorporating a wide variety of geological property information into the 3D geological model. Thus, it is well-suited to produce detailed 3D geological models attributed with physical, chemical, engineering or hydrogeological parameters, and intuitively analyze property characteristics within each modeled unit and their spatial relationships in 3D. This could dramatically improve the efficiency of exploring relationships and correlations hidden behind the complex and large volume of geological data fields, leads to an increased comprehensive understanding of the engineering geological space, and maybe produce new geological knowledge and promote new discoveries.

Although our attempts have been made to make the above-mentioned modeling framework as easy as possible for the creators and end users of 3D geological models, the concrete operations and applications of the coupled modeling method specifically designed for dealing with the increasing subsurface information are still undergoing modification. Based on our current work and research needs, we believe that at least four priority aspects need further research and development in the future: (1) geostatistical toolboxes (like GISLIB and

Fig. 5. Comparison of 3D property models for the spatial distribution of PCE: (A) result of the inverse distance weighted interpolation in the entire 3D space, omitting any structural constraint. (B) Result of the Ordinary Kriging method in the entire 3D space, omitting any structural constraint. (C) Result of the inverse distance weighted interpolation, guiding by the shape of the control strata predefined by 3D stratigraphic model.

TPROGS) to implement geostatistical analysis and simulation of spatial distribution of geological fields; (2) 3D visually analytic tools for coupled models; (3) quantitative spatial analysis techniques for multiple data fields; and (4) a readily applicable 3D modeling system which is specifically designed for the coupled modeling in engineering geological space. Our future work will consider how this functionality can be implemented through a collaborative, interdisciplinary research team consisting of geoscientists, computer scientists and geotechnical engineers.

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