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Conceptualization and characterization of envirochemical systems

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Abstract Reliability and uncertainty in groundwater model predictions is tied to the correctness of the conceptualization of the simulated system. The purpose of this paper is to present an integrated, stepwise approach for the conceptualization and characterization of subsurface envirochemical systems, building on the hydrological characterization approach developed by Kolm (1993). In the context of this paper, an envirochemical system is a subsurface hydrogeological and hydrochemical system containing chemical species of concern to environmental management. The conceptualization and characterization process, which is iterative and used at any scale, includes: (a) problem definition and database development; (b) preliminary conceptualization; (c) anthropogenic characterization; (d) surface characterization; (e) geological, geomorphic and geochemical characterization; (f) hydrogeological characterization; (g) groundwater flow system characterization and quantification; and (h) envirochemical system characterization and quantification. This approach may be used in: (a) evaluating natural variations in groundwater flow and envirochemical systems; (b) evaluating anthropogenic stresses on groundwater flow and envirochemical systems, such as pumping for water supply, irrigation, induced infiltration, or well injection; (c) evaluating presence and velocity of groundwater contaminants; (d) designing and selecting mathematical, geochemical, or transport models to simulate groundwater flow and envirochemical systems; (e) completing model schematization and attribution based on the problem defined, characterized groundwater flow and envirochemical system and model(s) selected; and (f) designing groundwater remediation systems.

INTRODUCTION

Reliability of groundwater model predictions typically depends on the correctness of the conceptual model, the availability and quality of model data and the adequateness of the predictive tools. This paper describes an integrated, stepwise method for the qualitative conceptualization and quantitative characterization of natural and anthropogenic subsurface envirochemical systems. A subsurface envirochemical system is a hydrogeological and hydrochemical system containing chemical species of concern to environ-

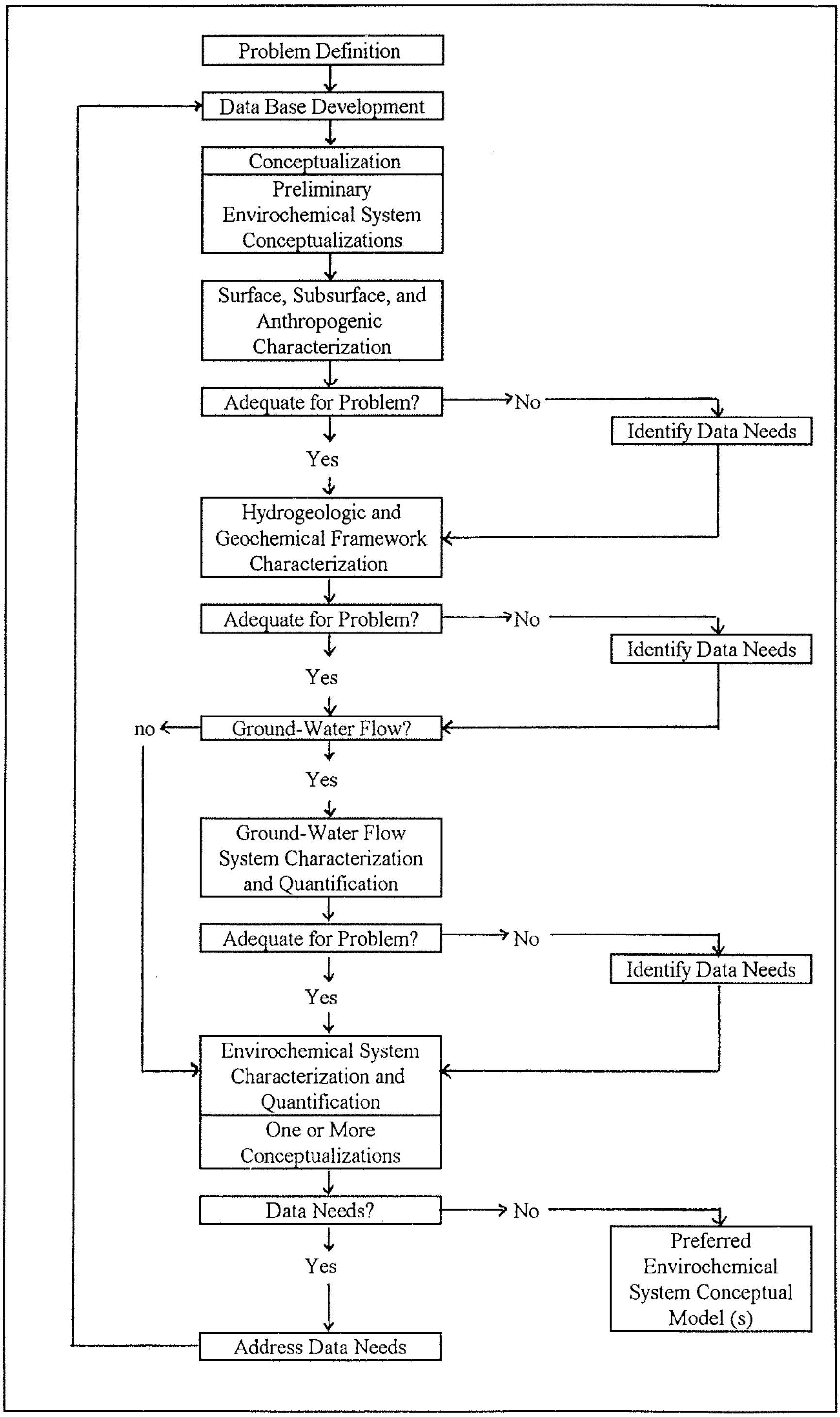

Fig. 1 Procedure for conceptualization and characterization of envirochemical systems.

mental management. It comprises the general concepts of the hydrological and hydrochemical system elements, active physical and chemical processes, sources and stresses, and the interlinkages and hierarchy of elements and processes with respect to the assessment of type, quantity, distribution and evolution of chemicals as influenced by soil, rock and water properties. The conceptualization and characterization process consists of systematic description and analysis of envirochemical system components, including: (a) problem definition and database development; (b) preliminary conceptualization; (c) anthropogenic characterization; (d) surface characterization; (e) geological, geomorphic and geochemical characterization; (f) hydrogeological characterization; (g) groundwater flow system characterization and quantification; and (h) envirochemical system characterization and quantification (Fig. 1).

Envirochemical system conceptualization and characterization is an iterative process for developing and attributing multiple working hypotheses (Fig. 1). The process starts with the development of a preliminary understanding of the envirochemical system based on project objectives, chemicals of concern and general physical and chemical principles and is followed by data collection and refinement of the understanding. Additional data collection and analysis and subsequent refinement of the conceptual models occur during the envirochemical model development and use, as required (Fig. 1). This process aims at reducing uncertainty in the formulation of alternative hypotheses derived from observation, interpretation and analysis, and in the final characterized and quantified conceptual model. This paper does not address the specific methods for characterizing envirochemical, hydrogeological and groundwater system properties, nor the quantitative uncertainty associated with specific methods of envirochemical, hydrogeological and groundwater system characterization and quantification.

The approach presented in this paper can be used at any scale and for any problem related to a particular envirochemical system. The approach is independent of the manner in which the problem may be solved, or the tools used in the design of the solution, including modelling. The nature of the problem to be solved will determine the type and scale of data collected and influence the specific results of each analysis.

Conceptualization and characterization are fundamental steps of envirochemical and groundwater flow system modelling. This overall process of modelling is similar to the modelling processes described by Anderson & Woessner (1992), Zheng & Bennett (1995) and Kolm *et al.* (1996).

After conceptualization and characterization are sufficiently complete to meet project objectives, the conceptual model may be translated into a mathematical model. Such a mathematical model typically consists of a set of governing equations and boundary conditions for transport simulation, or the equations describing chemical reactions with or without chemical and physical constraints. Relating such a mathematical model to a particular system requires specific values for system parameters, stresses and boundary conditions as well as rate coefficients. The conceptualization and characterization process is optimized when these inputs are identified early.

The application of geochemical and transport models requires making simplifying assumptions with respect to system processes, stresses and geometry, a procedure referred to as model schematization. Efficient model schematization starts early on in the conceptualization and characterization process and continues into the code selection, model design or construction and model attribution and calibration phases of a modelling project. In this paper, discussion regarding model schematization is focused on aspects of importance to the conceptualization and characterization process as is typically reflected in the problem definition or project objectives.

This approach may be used for project planning and data collection, but does not provide specific details of field characterization techniques. Refer to Tinsley (1979); Thornton (1983); Boulding (1991; 1993a; 1993b; 1994; 1995); and Sara (1994) for further guidance regarding field characterization techniques.

CONCEPTUALIZATION AND CHARACTERIZATION PROCESS

Problem definition and database development

First, the objectives of the project and the required or anticipated level of effort are defined. At this stage, the chemicals of concern may be identified and regulatory requirements considered. Once the project objectives and constraints are defined, the appropriate facets and scale of the envirochemical system for characterization are identified. This is followed by the determination of the study site boundaries using one or more of the following considerations: (a) natural site characteristics (topography, soils, geology, hydrology, biota, chemistry); (b) current and past land use and ownership; or (c) known or suspected extent of site-related contaminants. If site boundaries are initially defined by ownership, natural site characteristics should be evaluated to determine whether the scope of at least parts of the investigation should include areas that are off-site. For example, investigations of groundwater contamination should include areas of potential sources up-gradient and potential migration paths down-gradient from a site.

Data from existing sources are gathered by locating data sources and collecting and organizing relevant data into a manageable database. During this procedure data in the form of maps, tables and reports are collected from available published and unpublished sources. Furthermore, data from published or unpublished field studies are gathered and the methods used to collect and analyse the data are noted. Also, data from published or unpublished laboratory studies are collected. For each of these types of data, the methods used to collect and analyse the data and the levels of quality assurance and quality control, as required by the project, are noted.

Preliminary conceptualization

Preliminary qualitative envirochemical system conceptualization and field reconnaissance are conducted using the data bases developed during the problem definition and data base development step. Transforming data into a conceptualization is a rather intuitive process consisting of: (a) qualitative and quantitative data interpretation of individual data elements and grouped data within a particular data type; (b) analysis of spatial and temporal relationships between various data types; and (c) relating data types and interpreted data to elements of the specific envirochemical system (i.e. processes, structure, state and stresses). This process may be enhanced by comparison with previously conceptualized systems (i.e. role of experience). This approach results in the development of one or more initial conceptual models that will be used for further characterization and quantification. During this procedure, anthropogenic, surface and subsurface (geological, geomorphic, geochemical) features of the study area and chemical constituents, hydrogeological and geochemical framework, groundwater flow system and envirochemical system are characterized qualitatively. The resulting conceptual model of the envirochemical system includes a qualitative assessment of how chemicals enter, move through or are retained in and leave the envirochemical system. The source, transport, fate and resulting distribution of each targeted chemical (e.g. inorganic and/or organic chemical constituents, tracers and isotopes) in the envirochemical system are conceptualized at this time, or, in the case of unknown sources, source locations and strengths are hypothesized from the conceptualized transport and fate processes and the actual distribution of chemicals.

The envirochemical system conceptual model(s) is(are) described and visualized using cross-sections and plan view illustrations. This envirochemical system conceptual model may be modified at any stage of quantitative characterization (Fig. 1).

Anthropogenic characterization

The next step, anthropogenic characterization, includes determining type, distribution and rates of anthropogenic chemical processes and type and distribution of substances in the surface and subsurface (see Boulding, 1995, for guidance). Analysis of anthropogenic-related envirochemicals includes, but is not limited to, industrial, municipal/urban, domestic, agricultural and mining/resource related releases and uptakes.

At this time, the analysis of the type, distribution and amount of the targeted chemical species will reveal if subsurface flow is an important process. If the targeted chemical species has moved, it may be necessary to conceptualize and characterize the groundwater flow system, including hydrogeological and groundwater system characterization (Fig. 2) (Kolm *et al.*, 1996).

Surface characterization

Surface characterization, including type, distribution and amount, of natural chemical processes and substances at or near ground surface, is conducted (see Drever, 1982; Ritter, 1994; and Boulding, 1995, for guidance). During this procedure studies regarding vegetation-related (including plant releases and uptake), surface water-related (streams, lakes/wetlands, ocean and springs/seeps) and climate-related (snow, rain, fog) chemical exchanges with the subsurface system are conducted. The physical and chemical processes and resulting mass exchanges across the surface are characterized during this step.

Geological, geomorphological and geochemical characterization

Geological, geomorphological and geochemical characterization is conducted, including determining type, distribution and amount of natural chemical processes and substances in the subsurface (see Krauskopf, 1979; Berner, 1971; Stumm & Morgan, 1981; and

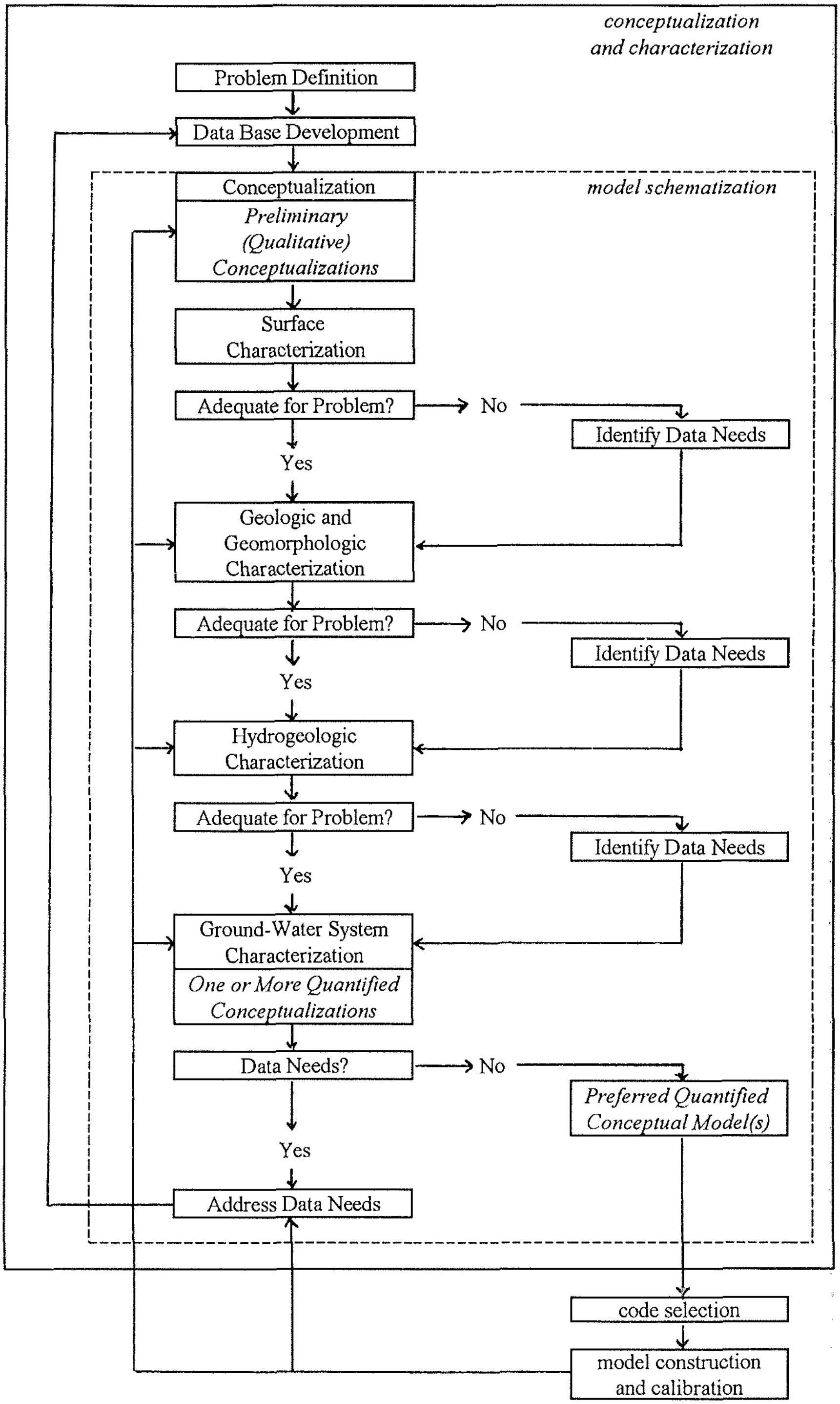

Fig. 2 Procedure for conceptualization and characterization of groundwater systems. (from Kolm *et al.*, 1996).

Boulding, 1995, for guidance). During this procedure, the petrological, mineralogical and geochemical factors and compositions are analysed with respect to spatial and temporal variations caused by geological (igneous, metamorphic and sedimentary) and geomorphic processes. This includes an analysis of the original chemical form and the evolution of solid geochemistry with time.

The geomorphological processes and deposits pertinent to the characterization of envirochemical systems include weathering and paedogenesis (e.g. soil horizon texture and chemical effects), mass wasting (colluvium textures and chemistry), fluvial activity (alluvium textures and chemistry), aeolian activity (dunes texture and chemistry), glacial activity (e.g. moraines, till and outwash plain textures and chemistry), coastal activity (beach and lagoon materials texture and chemistry) and anthropogenic features (e.g. road fill, tailings piles, foundation material texture and chemistry). The geological processes pertinent to the characterization of envirochemical systems, including the sedimentary, igneous and metamorphic processes and the resulting rock materials are evaluated and an analysis of the original chemical form and the evolution of solid geochemistry with time is performed. The spatial and temporal distribution of these geological materials is based on the principles of mineralogy, petrology, geochemistry, stratigraphy (depositional environments and lithology) and structure of the geological units. Geological maps and cross sections, subsurface investigation logs and stratigraphic columns are used, in conjunction with surface characterization, geophysical data and analysis, and geochemical data and analysis, to develop a part of the geological and geochemical framework that represents the distribution of lithological units and mineralogical and geochemical compositions as envirochemical system materials. Finally, the subsurface fluids (e.g. vadose zone fluids, groundwater and soil vapour) are characterized for envirochemical behaviour, including the reactions between subsurface fluids and matrix materials. Again, the chemical processes are transient in nature and need to be characterized on a temporal and spatial basis.

Hydrogeological characterization

Hydrogeological characterization consists of three phases: (a) identification and characterization of the hydrostratigraphic units; (b) identification and characterization of the hydrostructural units; and (c) combining hydrostratigraphic units and hydrostructural units into a set of hydrogeological units. Each hydrostratigraphic, hydrostructural and hydrogeological unit is defined as a discrete volume element of the subsurface geological framework. General discussion regarding groundwater processes is available in Freeze & Cherry (1979) and Fetter (1994); extensive discussion regarding the hydrogeological characterization procedure is available in Kolm (1993) and Kolm *et al.* (1996).

Groundwater system characterization and quantification

The groundwater system is characterized and quantified by determining the type, amount, temporal variation and spatial distribution of groundwater recharge and discharge using surface, subsurface and hydrogeological analysis. Furthermore, reaction and flow paths of indicative chemical species are analysed for information regarding the groundwater flow system. The groundwater system is quantitatively defined in terms of boundary conditions, flow paths and potentiometric surfaces and groundwater system budget (see Engelen & Jones, 1986; Domenico & Schwartz, 1990; Anderson & Woessner (1992); Kolm, 1993; Boulding, 1995; and Kolm *et al.*, 1996 for additional guidance). Exploratory groundwater modelling of one or more conceptual models, particularly the matching of the results of numerical models with observations of heads and fluxes, may be used for the quantification of the hydrodynamics of the characterized groundwater system, for checking the groundwater flow system characterization for deficiencies (conceptual model or attributes) and for determining subsequent field sampling programmes.

Envirochemical system characterization and quantification

The natural and anthropogenic surface or subsurface origins of targeted chemical constituents are characterized and quantified, including type, spatial and temporal distribution and amount. The presence, transport and fate of these chemical species, including form and spatial and temporal distribution, is characterized and quantified using the information obtained in the previous steps. At this time, relevant physical and chemical processes of the envirochemical system are mathematically described and quantitatively attributed. Processes of interest include, but are not limited to: (a) advection; (b) adsorption; (c) dispersion; (d) molecular diffusion, (e) volatilization, (f) hydrolysis; (g) oxidation/reduction; (h) chelation; (i) ion exchange; and (j) dissolution/precipitation and biotransformation (see Zheng & Bennett, 1995; Appelo & Postma, 1993; Domenico & Schwartz, 1990; Dragun, 1988; and Thornton, 1983, for additional guidance). The final result of this analysis is a characterized and quantified preferred envirochemical system model(s) (Fig. 1).

Upon completion of the conceptualization and characterization process, an adequate computational procedure is chosen, often in the form of a geochemical or transport computer code (Appelo and Postma, 1993; Zheng and Bennett, 1995). After selecting a particular computer code, the model construction phase is entered where code-specific aspects are addressed, followed by model calibration and sensitivity analysis during which the conceptual model may be revisited (Fig. 1).

CONCLUSIONS

In many projects dealing with the distribution of hazardous chemicals in the subsurface, decisions are made without obtaining a thorough understanding of the extent, complexity and hierarchical nature of the affected system. Thus it often occurs that important elements of such a system are not studied to the extent necessary to obtain optimal solutions. To address this issue, the conceptualization and characterization process described in this paper has been developed. It takes a top-down, hierarchical approach to envirochemical system analysis, ensuring that all elements, processes and constraints of the envirochemical and hydrological systems involved are addressed and properly evaluated at a level of detail commensurate with project objectives and constraints. As this conceptualization and characterization is aimed at solving real-world problems, the nature of these problems and specific management requirements in addressing them provide important guidance at different stages of the process.

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