SCS: Specific Chemical Simulators dedicated to chemistry-transport coupled modelling: Part II. A simplified coupled modelling approach based on Networks of Chemical Reactors (NCR)

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As highlighted in part I of the present abstract, the study of pollutant migration in natural systems requires to use coupled chemistry-transport modelling. In this abstract, we present a simple coupling approach based on the concept of Networks of Chemical Reactors (NCR). This approach is inspired after the reactor assembling method described by Villermaux (1982) and widely used for chemical process modelling.

Outlines of the NCR approach

The basic assumption in the NRC approach is that the studied medium constitutes an integrated biogeochemical and hydrodynamical system. First, the physical boundaries of the system are defined. Secondly, the structure of the NCR is designed on the basis of biogeochemical and hydrodynamical characteristics of the system. Each individual reactor in the NCR is a conceptual building block related to a specific area of the total system.. Reactors are defined by their positioning within the flow path network, by their volume, and by their initial content (solid and aqueous phases) as indicated on Fig. 1.

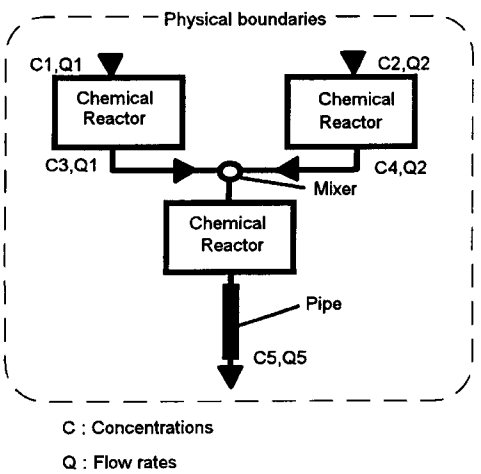

FIG. 1. General structure of a NCR.

The hydro-transport processes are restricted to advection and mass transfer between connected reactors. Because of its flexibility, this simplified coupled modelling approach can be applied to a wide range of field of investigations (flow cell experiments, process engineering, mining pollution,...). Other codes based on the same principles exist in the literature. IMPACT (Jauzein *et al.*, 1989) is one of them. The ground bases for the application of this NCR approach to water pollution problems related to mining were established at BRGM by Altmann (1995).

Specific BRGM methodology for NCR design and construction

We presented in part I of the present abstract an original method for designing Specific Chemical Simulators (SCS). The SCS constitutes the core of the chemical reactor. This means that our strategy in designing NCR also relies on the use of the ALLAN-NEPTUNIX 4 modelling tool. Therefore, we directly benefit of the user-friendliness and the modularity offered by the ALLAN-NEPTUNIX 4 package. Once the SCS is available, the reactors and NCR construction tasks are then limited to a simple graphical assembling.

A chemical reactor is composed of several modules as indicated on Fig. 2: an SCS (see detailed description in part I of present abstract); an Hydrological module (*H*) which is based on a relation between head and flow rate. In the case of a porous medium, this relation is given by Darcy's law; several Transport modules (*Ti*) related to each of the *i* chemical elements considered. The basic equation solved in each of these modules is the molar flow rate balance of element *i*. This equation contains a source/sink term which is calculated in the SCS.

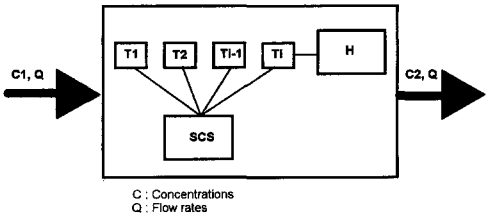

FIG. 2. General ALLAN structure of a chemical reactor.

Once all of the required reactors are constructed following the methodology presented above, the construction of the NCR consists in a graphical assembling, according to the previously established system flowsheet, of all the individual reactors using connection elements such as pipes, mixers, and splitters. Except the SCS, all of these modules are totally system-independent ; so they are stored in our model library and then can be re-used without any code writing effort for future applications.

The complete NCR set of equations (hydrodynamic, transport, and chemistry) leads to the automatic generation by NEPTUNIX 4 of a unique large squared matrix. Consequently, the whole set of equations is solved simultaneously at each time step, contrary to many other coupled codes in which chemical and transport calculations are done in two steps (cf. Kervévan *et al.*, part III of present abstract). The NCR approach enables us to better simulate strong coupling between the various processes.

Another advantage of the BRGM NCR approach is that any of the reactor modules can be readily modified or replaced. For instance, assuming that a law between porosity and permeability variations is known, it is very straightforward to implement this law in the *H* module and to simulate the plugging of a chemical reactor due to mineral precipitation (porosity being related to amounts of precipitated minerals calculated in the SCS) and its influence on flow.

Example of case study

The applicability of the NCR approach was tested at BRGM in a variety of studies, such as reactive tracer column experiments interpretation or process engineering modelling. As an illustration, we report herein an example dealing with heap leaching of gold. Because of the chemical and hydrodynamical complexity of this leaching process and the lack of knowledge of many key parameters, we first chose to use the NCR modelling approach in order to determine the critical parameters of the system. The NCR has to be considered in this case as an interpretation aid tool and not as an ultimate and predictive model.

In this study, the heap was arbitrarily divided in two reactors. We present two calculated curves showing the variations with time of $AuCN_2^-$ and dissolved oxygen (O_2(aq)) content in each reactor (Fig. 3) for given chemical and hydrodynamical conditions.

Conclusions

The NCR approach combined with the use of ALLAN and NEPTUNIX 4 softwares provides a very flexible tool for modelling the behaviour of integrated biogeochemical and hydrodynamic systems. This approach can be adapted to various site complexity levels and to the representation of all-level relevant information. In most cases, it must be considered as an interpretation or/and a decision aid tool.

References

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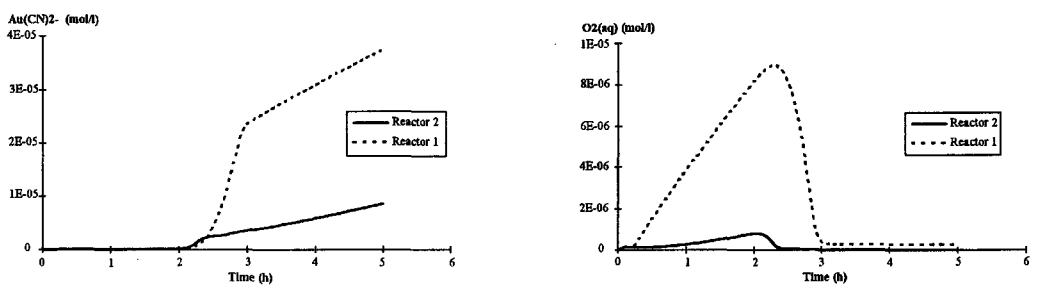

FIG. 3. Variations with time of $AuCN_2^-$ and O_2(aq) content in each reactor.