Testing Online Collaboration on Trace Metal-Humic Binding Modelling

Montserrat Filella

SCHEMA, Rue Principale 92, L-6990 Rameldange, Luxembourg, filella@schema.lu

Keywords: humic, fulvic, natural organic matter, metal binding, complexation constants, models

1. INTRODUCTION

Ten years ago, W. Hummel, in one of the best reviews ever published on binding models for humic substances, described the situation faced by any modeller as a “veritable jungle” [1]. The situation is even worse for any potential model user freshly embarking in the field or for any scientist who simply wishes to gain an understanding of the scientific literature. Reading the many reviews that exist on the subject may be very useful to all the potential ‘explorers’ of this jungle, whether modellers, users or ‘outsiders’, but these reviews are sometimes difficult to follow, often lack the practical details indispensable for practical applications, and are unavoidably biased by the subjective appreciation of the ‘expert’ who wrote them. Thus, review papers alone rarely provide the complete picture.

It is important to note that such a myriad of models exist not because of the caprices of model developers. Rather, this stems from the fact that the nature itself of the trace element binding properties of humic-type substances severely hampers description: they are undefined complex mixtures of organic compounds that defy the rules commonly applied to other types of chemical substances. This has the serious consequence that, in all probability, there will never be a universal, definitive model and that humic-binding models are ‘empirical’ by nature, their usefulness finally being directly related to their ability to solve particular problems. Scientists trained in disciplines where mechanistic models, based on first-principles, are highly praised find this fact difficult to accept.

Choosing the most appropriate model for solving a particular problem may be facilitated by taking an evidence-based approach, similar to those developed in the medical sciences [2,3]. This path has rarely been explored in environmental sciences. It requires clear information about the existing approaches and access to the models. The online collaboration described here will hopefully be a first step in this direction.

2. TRACKING AND ARCHIVING MODELS

Most of the models described in the literature require specific computer applications in order to be applied. In practice, however, most of these applications are now unavailable. Various factors have led to this situation:

In: From Molecular Understanding to Innovative Applications of Humic Substances; Proceedings of the 14th International Meeting of the International Humic Substances Society, September 14-19, 2008, Moscow – Saint Petersburg, Russia, Editors: I. V. Perminova, N. A. Kulikova, Vol. II, Humus Sapiens, Moscow, 2008, pp. 405-408.

- Although code obsolescence is a problem faced in many different environments (business, government, academia, etc), it is particularly serious in the academic world where the economic incentive to upgrade programs is lacking and where know-how is often lost due to the complexities of the academic world.

- Some models were intended to be used only once. A typical example would be the “oligotroelectrolyte model” developed by Bartschat and co-workers [4]. This model has been abundantly cited (146 times according to the Web of Knowledge) and described in virtually every review on the subject but, to our knowledge, it was used only once to produce the original publication. It probably constitutes a perfect example of the halo effect of scientists working in high-prestige institutions [5,6].

- Most of the models never had a finished, optimized version. Computer code is usually developed as part of a PhD thesis or project and used only by the developer and a limited number of collaborators. Often, user-friendly and well-documented copies are never produced and distributed.

The result is that (i) an incredible amount of scientific knowledge is in fact lost; (ii) only readily-available models are used in practice, irrespective of their actual value and suitability with regard to the problem that needs to be solved; (iii) significant amounts of time are lost reinventing the wheel.

The collaborative web portal being developed contains links to available code and may act as a repository for any existing program. An ’open source‘ approach whereby obsolete code is made available to be improved will be used, subject to the approval of the original developers.

3. A COLLABORATIVE WEB PORTAL THE WIKI WAY

The scientific literature describing and modelling trace element binding by NOM includes four types of publications: (i) original publications where the model is initially described by the developers and possibly modified later; (ii) applications of the models by end-users; (iii) papers comparing models; (iv) review papers. As mentioned above, finding one’s way through this ‘jungle’ is far from straightforward. Many traps are lying in wait for the unwary:

- Often models are published without having undergone the necessary validation process. Over time, mistakes are discovered (or the repeated use of the code reveals some shortcomings) and, hopefully, corrected. This process produces a saga of articles where the logical thread is difficult to follow and from which misunderstandings easily

arise. For instance, just such a situation recently prompted the developers of a popular model, the NICCA-DONAN model, to devote an entire paper to clarifying the situation [7].

- In the cases where the code is available, the developers' help is needed to apply it correctly. At least, a quick review of the applications of Model VI-WHAM [8] and the NICCA-DONAN model [7] in a well-known journal, Environmental Science and Technology (years 2002-2007) shows that in a significant percentage of the articles where these models are applied, either the developer appears as an author or the study has been performed in close connection with his lab.

- By nature, model developers always think that their own models are the best and an objective exchange of experiences becomes difficult.

The above considerations mean that an online portal where information is contributed and updated by the developers themselves and the users would be extremely valuable. However, this is difficult to achieve through the traditional channels of scientific communication (conferences, peer-reviewed articles) because of their lack of 'reactivity' and limited audience. New collaborative tools such as wikis may provide a better platform. A wiki is a type of website that can be directly edited by visitors using only their web browser. Wikis are useful for collaborative document creation because document viewing and editing are integrated on-line. The changes to the wiki are stored in a database on a web server and are immediately visible to visitors. A record of all changes is also stored in the database so that older versions of the site's pages can be restored. The construction of a wiki on humic binding modelling may help to establish a neutral, permanently updated reference.

4. FOLLOW-UP OF THE LITERATURE THE BLOG WAY

New applications of existing models continuously appear in the scientific literature. Comprehensive follow-up is difficult and, in all probability, not worthwhile. Publication of reviews and compilations is time-consuming and relatively slow. Moreover, personal opinions and experiences cannot always be adequately reflected in such publications. An experiment is underway whereby new publications will be spotted and referenced and, if deemed interesting, commented on in a blog. The very nature of such coverage means it makes no claim to being comprehensive and the contents will be, to a certain extent, subjective. Information on 'buried' ideas and papers will also occasionally be commented on. The overall objective is to stimulate feedback and the exchange of experiences in the 'humic binding community'.

REFERENCES

1. Hummel, W. 1997. *In*: Modelling in Aquatic Chemistry, I. Grenthe and I. Puigdomenech (Eds.), Nuclear Energy Agency, Paris, pp. 153-206.
2. Sackett, D.L., Rosenberg, W.M., Gray, J.A., Haynes, R.B., Richardson, W.S. 1996. BMJ 312, 71-72.
3. Elstein, A.S. 2004. Inflamm. Res. 53 Suppl 2, S184-S189.
4. Bartschat, B.M., Cabaniss, S.E., Morel, F.M.M. 1992. Environ. Sci. Technol. 26, 284-294.
5. Cole, J.R., Cole. S. 1972. Science 178, 368-375.
6. Cole, J.R., Cole. S. 1973. Social Stratification in Science. University of Chicago Press, Chicago.
7. Koopal, L.K., Saito, T., Pinheiro, J.P., van Riemsdijk, W.H. 2005. Coll. Surf. A 265, 40-54.
8. Tipping, E. 2002. Cation Binding by Humic Substances. Cambridge University Press, Cambridge.