

Kinetic-based model for mixed weak acid/base systems

EV Musvoto, MC Wentzel*, RE Loewenthal and GA Ekama

Water Research Group, University of Cape Town, Department of Civil Engineering, Rondebosch, 7700, South Africa

Abstract

This paper describes the development of a simple kinetic model for mixed weak acid/base systems. In the model, the weak acid/base equilibria are formulated in terms of the kinetics of the forward and reverse reactions for the dissociation of the weak acid/bases. The parameter (compound) H^+ is also explicitly included in the model, so that pH can be calculated directly. The weak acid/bases included are water, carbonate, ammonium, phosphate and short-chain fatty acids. However, the approach used to develop the model is general, and can be applied to include any other weak acid/base of importance. Precipitation of $CaCO_3$ and gaseous exchange of CO_2 also have been included. The model and the approach on which it is based have been validated by comparing model predictions to those obtained from equilibrium chemistry-based models; good correlation was obtained. Compared to the equilibrium chemistry approach to modelling mixed weak acid/base systems, the kinetic approach offers several advantages. In particular, the use of kinetics will facilitate integration of the weak acid/base model with other kinetic models (biological, chemical or physical). For example, the model presented here can be readily integrated with the existing biological kinetic models for wastewater treatment systems, to extend application of these models to situations where an estimate for pH is essential. Furthermore, by providing an estimate for pH and for the species making up the weak acid/bases, the model will simplify inclusion of chemical and physical processes, where these are of importance.

Introduction

To aid the design and operation of, and research into, conventional biological waste-water treatment systems, a variety of mathematical models has been developed. With few exceptions, these models have focused almost exclusively on the biologically mediated processes that lead to the removal of, or change in, the particular compounds of interest. For example, models for the activated sludge system have progressively included the biologically mediated processes of COD removal, nitrification, denitrification and biological excess phosphorus removal (Dold et al., 1980; 1991; Van Haandel et al., 1981; Henze et al., 1987; Wentzel et al., 1992; Henze et al., 1995). In this group of models, by focusing on the biological processes usually it is implicitly assumed that;

- The biological processes dominate the system response; and that
- chemical and physical processes (e.g. precipitation and gas stripping respectively) play an insignificant role compared to the biological processes and accordingly can be neglected,
- compounds not directly involved in the biological processes or not of interest, even though present, do not significantly influence the behaviour, and
- the biological processes take place within a regime of constant pH.

This has restricted application of these models to situations where the assumptions remain valid. For the activated sludge system treating municipal or similar types of waste waters, where the organics are present at relatively high concentrations compared to the nutrient (N & P) concentrations, these assumptions usually are valid. For example, in the nitrification of municipal waste

waters it usually is reasonable to assume that the biological processes dominate and that there is sufficient buffer capacity present to absorb the generation of hydrogen ions (H^+) and loss of CO_2 so that the pH does remain approximately constant; some of the models have included the parameter "alkalinity" to check that this condition is in fact true (e.g. Dold et al., 1991). However, in the treatment of a number of waste waters the assumptions are not valid and the models cannot be applied. For example, in the nitrification of waste waters with low buffer capacity and/or high N concentrations, or in the treatment of waste waters where the generation or utilisation of short-chain fatty acids (SCFA), e.g. acetic, propionic, is significant, the assumption that the pH remains essentially constant no longer can be accepted.

In particular, the models cannot be applied to situations where chemical and physical processes do play a significant role, and so cannot be neglected. For example, one such category of waste waters is that where the organics are present at relatively low concentrations compared to the nutrients. These waste waters, termed high nutrient, low organic carbon, are generated in a number of municipal waste treatment operations such as trickling filter effluents, anaerobic digester supernatants, activated sludge dewatering liquors, landfill leachates, septic tank effluents and waste sludge lagoon effluents. In the treatment of these waste waters, chemical and physical processes can be expected to play a significant role and no longer can be neglected; these processes and their interactions with each other and with the biological processes will have to be included in any model of these treatment systems. In other words, a model integrating the biological, physical and chemical processes of importance will be required. Deterministic models that quantitatively describe the stoichiometry and kinetics of the biological processes are well advanced, e.g. IAWQ Model No. 1 (Henze et al., 1987; Dold et al., 1991) and No. 2 (Henze et al., 1995). Similar models need to be developed for the chemical and physical processes, and integrated with the biological models. Models including chemical and physical processes will require that the pH parameter/compound is incorporated and accurately determined, as pH is of fundamental importance in these processes, significantly

* To whom all correspondence should be addressed.

8 (021) 650-2583; fax (021) 689-7471; e-mail markw@engfac.uct.ac.za
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