Available online at www.sciencedirect.com

SCIENCE DIRECT®

Computers & Education 43 (2004) 81–90

COMPUTERS & EDUCATION

www.elsevier.com/locate/compedu

Using a laboratory simulator in the teaching and study of chemical processes in estuarine systems

E. García-Luque *, T. Ortega, J.M. Forja, A. Gómez-Parra

Dpto. de Química Física, Facultad de Ciencias del Mar y Ambientales, Universidad de Cádiz, Campus Río San Pedro s/n 11510, Puerto Real, Cádiz, Spain

Abstract

The teaching of Chemical Oceanography in the Faculty of Marine and Environmental Sciences of the University of Cádiz (Spain) has been improved since 1994 by the employment of a device for the laboratory simulation of estuarine mixing processes and the characterisation of the chemical behaviour of many substances that pass through an estuary. The equipment comprising the simulator is controlled by a computer system running the program OLE (Oceanography and LEarning), which was developed originally as a research tool in Chemical Oceanography (under Windows® environment). Later, on the initiative of several teachers, the handling of the simulator was simplified to allow its use as a didactic resource for teaching the various processes that take place in littoral systems.

Since its initial development, many different natural environmental conditions have been simulated, and the behaviour of many chemical pollutants has been studied. On the basis of this favourable experience, the simulator designed appears to be a versatile tool that can be usefully employed in both academic learning and research work.

Keywords: Applications in subject areas; Improving classroom teaching; Interactive learning environments; Simulations

1. Introduction

The teaching of advanced experimental sciences (specifically related to chemical oceanography) at the higher education level requires students to perform laboratory work as well as field practice. However, field surveys related to chemical oceanography present various practical difficulties.

* Corresponding author. Tel.: +34-956-016423; fax: +34-956-016040.
E-mail address: enrique.luque@uca.es (E. García-Luque).

doi:10.1016/j.compedu.2003.12.006

Estuaries are zones of intense biological and geochemical activity where significant amounts of matter and energy are exchanged with the ocean. Therefore, these systems present particular interest in the study and teaching of the chemistry of marine and environmental sciences. Learning activities in these sciences are difficult to carry out for several reasons (Ortega, Forja, & Gómez-Parra, 2001): they are expensive to organise; they require a lot of time and the participation of several teachers; they are difficult to coordinate with the rest of the learning activities during the course; and they are very dependent on weather conditions.

All these problems can be avoided, or minimized, by employing laboratory simulations. In this sense, without denying the need to work on site for this type of studies, simulations can significantly reduce the amount of field survey work to be carried out during an academic year. Logically, results obtained by means of simulation need to be validated by comparison with field measurements.

But, in addition, laboratory simulation offers other advantages over fieldwork: by controlling in the laboratory the desired environmental conditions, it is possible to reproduce certain processes that occur only sporadically or unpredictably in the field.

The idea of dynamic simulation is basically similar to that described by Bale and Morris (1981). Nevertheless, the dimensions and the features offered by these new simulators are considerably greater. The principal improvement consists of the remote control of the equipment by means of a computer system.

Simulations can be defined as computationally correct representations of a situation which offer the user control over the outcome of the program (Davies, 2002). In this respect, it is the students themselves who actively participate in their learning (Kearsley & Shneiderman, 1998). Thus, simulation allows multiple perspectives of knowledge and is of a complexity which approaches reality; engaged students feel a sense of ownership of the task, and practice metacognition (Davies, 2002).

Simulations have already been recognized as an efficient and effective way of teaching and learning complex, dynamic systems (Parush, Hamm, & Shtub, 2002). Efficiency is gained by reducing the time it takes to reach a specified level of learning, and effectiveness is gained by achieving better results in performing the tasks learned.

Specifically, two versions of our laboratory simulator have been developed in the Department of Physical-Chemistry of the Faculty of Marine and Environmental Sciences of the University of Cádiz (Spain). The first version was introduced in 1994 and an improved version was developed later. From the beginning of these laboratory experiments, both simulators have been used in practical teaching by more than 900 students, with very satisfactory results.

2. Description of the simulator

Basically, the simulation of estuarine mixing is achieved by the cross-current mixing of sea water with river water (Fig. 1). The mixture is performed in a series of eight tanks interconnected under a hydrodynamic regime and situated at ascending levels. The lowest tank is supplied with seawater, at a flow rate of Q_{SW}, and the highest tank is supplied with freshwater at a flow rate of Q_R. To each intermediate tank, i, a flow (Q_{i+1}) of higher salinity value is pumped from the tank immediately below it (using a peristaltic pump), while from it, by overflow, water is returned to

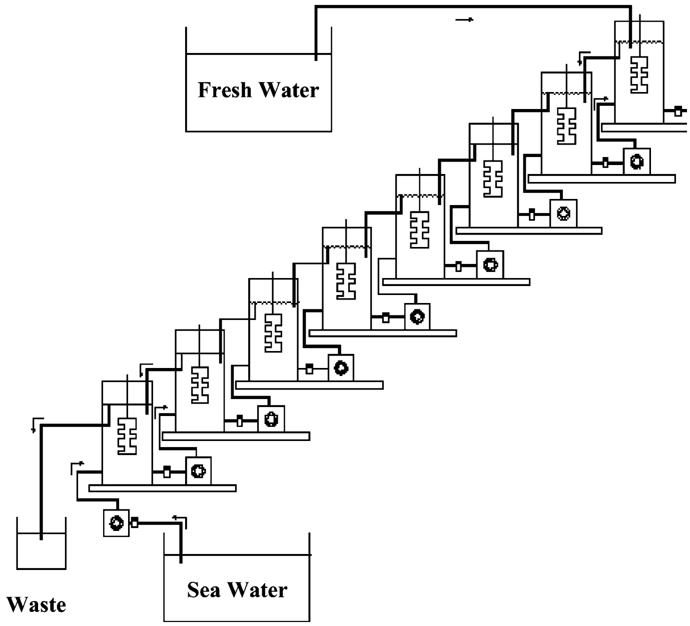

Fig. 1. Schematic representation of the estuarine hydrodynamic simulation system.

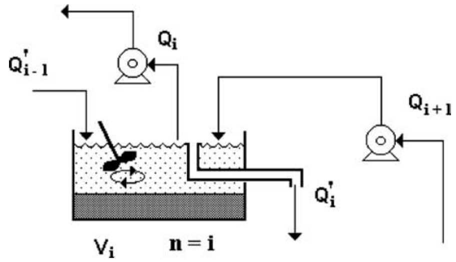

Fig. 2. Diagram of input and output water flows from each of the tanks comprising the simulator.

the same tank below at a flow rate of Q'_i. The intermediate tank also receives the overflow from the tank next above it (Q'_{i-1}), to which it in turn sends, by pumping, a flow of Q_i (Fig. 2).

The relationship between the salinity in each tank and the water flows between them can be established by means of a general and particular material balance (Eqs. (1) and (2), respectively)

$$Q_{i+1} + Q'_{i-1} = Q_i + Q'_i, \tag{1}$$

$$Q_{i+1} \cdot S_{i+1} + Q'_{i-1} \cdot S_{i-1} = (Q_i + Q'_i) \cdot S_i. \tag{2}$$

In which, for $i = 1$, $Q_{i-1} = Q_R$, and for $i = 8$, $Q_{i+1} = Q_{SW}$.

Solving the systems of Eqs. (1) and (2), it is possible to obtain a generic expression for the different flows necessary in each tank to simulate the expected salinity gradients

$$Q_i = Q_R \cdot \left[\frac{(S_{i-1} - S_R)}{(S_i - S_{i-1})} \right]. \tag{3}$$

So, by choosing appropriate relationships between the flows, it is possible to generate a large number of longitudinal salinity gradients similar to those of real estuaries. Conceptually, the simulation of the process of mixing in the estuary consists of substituting the continuous variation in salinity that is produced in a real estuary by a series of stages in each of which the salinity is constant, and between which there exists a sharp variation in the salinity.

The temperature in each tank is controlled by means of coated dip heaters. To ensure a homogeneous mixture of both types of water, variable-velocity mechanical stirrers are used. This feature provides vigorous agitation, which also keeps all the suspended particulate matter permanently in suspension. The tanks are aerated by means of a blower system, with submerged diffusers, to ensure the correct oxygenation of the water in all the simulations performed.

The initial version of the simulator was first used in 1994. A technical description of the device has been published by Ortega et al. (2001).

Later, in 1998, an improved version of the simulator was brought into use in the practical teaching of Chemical Oceanography. This second version of the simulator was adapted to make the system much easier for students to use. It was also necessary to develop a data acquisition system compatible with the technical characteristics of the devices that compose the system.

The data acquisition system consists of an AID 21-bits translation card that incorporates control loops to adjust the functioning of the system. Specifically, it is necessary to optimize the flow and temperature control of each tank comprising the simulator. Thus, flow and temperature control loops are intended to adjust real values of flow and temperature (achieved by means of peristaltic pumps and coated dip heaters, respectively) to their expected theoretical values. Regulation of flow involves setting up the peristaltic pumps (Masterflex, 7521–55) in phase with the flow-sensors (McMillan Co., 111), while temperature is monitored by thermistor probes and adjusted by means of coated dip heaters. The system is controlled by a program we have designated OLE (Oceanography and LEarning) specifically written in Visual Basic (under Windows® environment). The program OLE has been designed to be used as a part of the student exercises included in the Chemical Oceanography course. Fig. 3 shows a window with the three basic menu options: the flow and temperature control boxes and the calibration dialog box.

Under OLE, the computer keeps a continuous record over time of the different flows (supplied by the peristaltic pumps) and the temperature values in each tank. The A/D converter and the computer operate together providing a feedback control mechanism for the simulator. The system is able to correct flow or temperature values if necessary, adjusting them to the expected values.

The program OLE includes a PID control algorithm of velocity type. This algorithm is used for the control of almost all loops in the process industries and is also the basis for many advanced control algorithms and strategies (StClair, 1989). In order for control loops work correctly, the PID loops must be properly tuned. The PID control algorithm comprises three elements:

- Proportional, also known as Gain.
- Integral, also known as Automatic Reset or simply Reset.
- Derivative, also known as Rate or Pre-Act®.

The control loop that correctly manages the software of the system has three parameters, known as controller-tuning adjustments (K, gain; T_i: integral or reset time; T_d: derivative time).

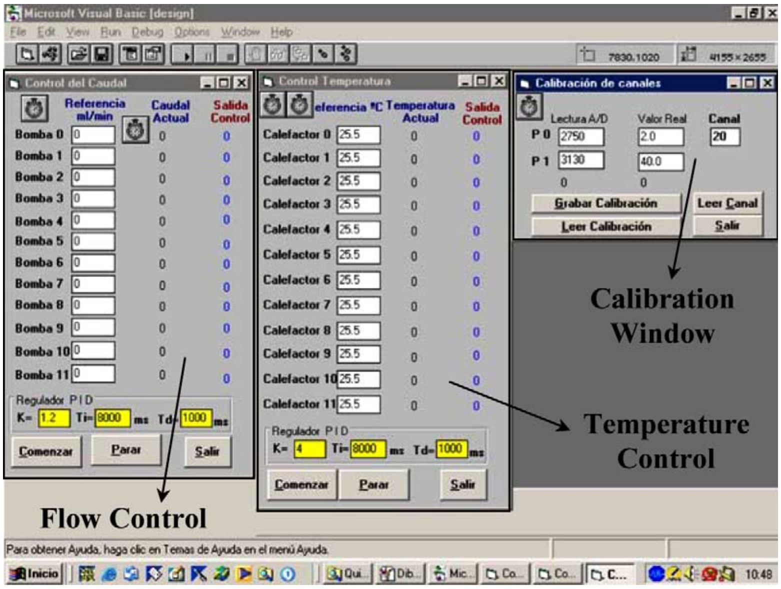

Fig. 3. Program window showing the three basic menu options of the program OLE: the flow and temperature controls and the calibration dialog box.

The PID algorithm must be tuned for the particular process loop controlled. This tuning is based on the dynamics of the process response. Therefore, by correctly varying these parameters simultaneously, flow and temperature control loops can be optimized.

Initially, before the start of any assay performed by pupils, it was necessary to carry out a series of checks in which control loop values were varied to find the most suitable ones for temperature and flow control. Thus, we concluded that optimum values in the case of flow control were: $K = 1.5$; $T_i = 4000$ ms and $T_d = 1000$ ms, while in the case of temperature control, these optimum values were: $K = 4$; $T_i = 4000$ ms and $T_d = 1000$ ms. Using these set of values, the lowest standard deviations due to differences between real values and expected values were obtained (for flow and temperature). Table 1 shows, by way of example, different expected flow values versus average recorded values for an assay of four days duration. In all cases, standard deviations were lower than 0.4% for real values achieved with the optimized control parameters, whereas standard deviations for real values achieved without the optimized control parameters were around 3%.

Table 1
Different expected flow values (mL min^{-1}) versus two types of average real flow values: with and without optimized PID parameters

Expected flow values (mL min^{-1})	Average real flow (with optimized parameters)	Averaged real flow (without optimized parameters)
15	15.040 ± 0.0542	15.010 ± 0.555
25	24.963 ± 0.0759	24.995 ± 0.582
35	34.999 ± 0.0290	34.958 ± 0.549
50	50.004 ± 0.0415	50.046 ± 0.765

Flows appear with their respective standard deviations. These laboratory assays had a duration of 4 days.

On the other hand, in different laboratory assays, it is necessary continuously to record the evolution of several variables like conductivity and pH in each tank. In such cases, it is necessary to employ another Personal Computer with the suitable software (an A/D converter) for correct data acquisition.

3. Results

Simulations were performed by students of a high level (4th year) course, in the subject: Physicochemical Processes at Littoral Systems, which is taught over a period of 16 weeks, with three hours of class contact per week (two sessions of 1 and 2 h, respectively). This subject has a heavy practical content. The objective of the simulations must be congruent with the objective of the learner, and must support the learner's objective (Davies, 2002).

Thus, the objective of the experiments performed was (i) to reproduce a longitudinal salinity gradient in the stationary state of a given estuary; (ii) to characterize the behaviour of several chemical species in their transit through this estuary.

The principal advantage of the described system consists of its versatility in producing any estuarine salinity gradient that students wish to simulate. They simply have to fix the salinity values that they wish to reach in each tank (similar to those found in the real estuary that they want to simulate). Then, they have to calculate the necessary flows (by means of Eq. (3)) to get that desired salinity gradient. The calculated flow values then form the input values for the OLE program. It is also necessary to input the desired temperature values for each tank (Fig. 3). Thus, the simulator makes it easy to reproduce a specific section of the real estuary employed like a model. It is feasible to check the accuracy of the simulator in relation to the creation of the salinity gradient by means of a mass balance, in which errors of more than 1% are not detected. Fig. 4 shows, by way of example, a plot that represents theoretically expected salinity values for each tank of the simulator versus experimentally measured salinity values obtained at the end of an experiment. The correlation coefficient ($r^2 = 0.992$) confirms the correct functioning of the setup during the experiments.

In relation to the behaviour of several chemical species in their transit along an estuary, students from different academic years have studied the behaviour of majority elements (Cl^-, Ca^{2+},

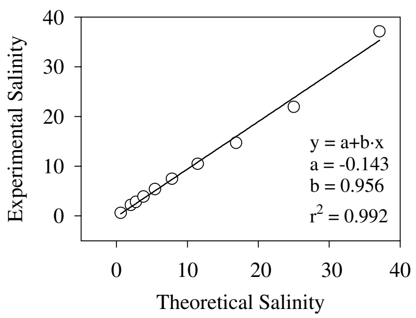

Fig. 4. Theoretically expected salinity values for each tank of the simulator versus experimentally measured salinity values obtained at the end of a laboratory experiment.

SO_4^{2-}), heavy metals (Zn, Cd, Pb, Cu), nutrients (NO_3^-, HPO_4^{2-}, SiO_2) and gases (O_2, CO_2), by applying the ‘‘Reactant Method’’ (Morris, 1985). Samples are collected directly by the students from each of the tanks of the simulator. For this, peristaltic pumps and other systems of the simulator are stopped by means of the Personal Computer for around one hour before each sampling (to eliminate any over-saturation of the dissolved gases). Analytical techniques employed to quantify the concentrations of the different compounds analysed have been described by Grasshoff, Ehrhard, and Kremling (1983). Some of the results obtained on different courses are shown in Fig. 5. This figure shows four plots of different elements (specifically, a heavy metal, a majority element, a nutrient and a gas) along a simulated salinity gradient.

Thus, Fig. 5 shows a linear relationship between the concentration of Ca^{2+} (in the dissolved phase) and the salinity. This conservative behaviour is also observed for the other majority elements in the sea water. On the other hand, nutrients can display different behaviours in function of their reactivity. For example, phosphate in the simulator (Fig. 5) is non conservative. This result, which also is in agreement with those obtained in field studies (e.g., Lebo, Sharp, & Cifuentes, 1994), may be attributed to apatite formation (generally in areas of low salinity values). Similar behaviour is shown by metals. Fig. 5 shows evolution of the reactivity of Zn along a salinity gradient. This reactivity is related to adsorption processes onto the suspended particulate matter of both organic and inorganic origin. In fact, there is a considerable body of field evidence supporting this statement, dating from several years ago (e.g., Wood, Baptista, Kubawara, & Flegal, 1995, etc.). On the other hand, partial pressure of CO_2 measured in a laboratory experiment shows a similar behaviour to that described by Frankignoulle et al. (1998) in field surveys.

Therefore, in the simulations carried out by the students, the types of behaviour of the analysed compounds coincided with those expected in the field. As an example, the concentrations obtained

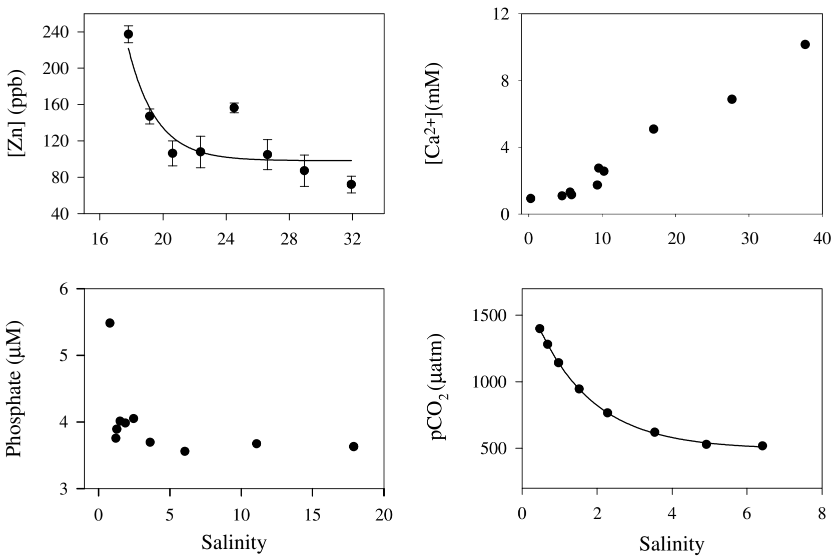

Fig. 5. Variations of the concentration of Zn (ppb), Ca^{2+} (mM), PO_4^{3-} (µM) and pCO_2 (µatm) over different salinity gradients, in several laboratory experiments carried out by the students.

Table 2
Concentration ranges for Zn, Ca^{2+}, PO_4^{3-} and pCO_2 obtained in several natural estuaries

	Range	Estuaries	Reference
Zn (ppb)	[25–200]	Guadalquivir	Gómez-Parra, DelVAlls, Forja, Sáenz, and Riba (2000)
Ca^{2+} (mM)	[1–10]	Volga	Burton (1976)
PO_4^{3-} (μM)	[0.5–5.0]	San Francisco Bay	Smith, Peterson, Hager, Harmon, Schemel, and Herndon (1985)
PCO_2 (μatm)	[465–2800]	Gironde	Frankignoulle, Abril, Borges, Bourge, Canon, Delille, Libert, Théate, (1998)

for these compounds (Fig. 5) were of the same orders of magnitude as the concentrations quantified in natural estuaries (Table 2).

Despite the student's lack of analytical experience (the use of the simulator involves some degree of error), the results obtained have generally been satisfactory.

Improved version of the simulator even offers the possibility of simulating tidal regimes. Innovations intended for future courses include the simulation of different tidal regimes, which will also contribute to familiarising students with the use of the simulation for research.

3.1. Evaluation of the simulation

This estuary simulator was developed originally as a research tool in chemical oceanography. Then, on the initiative of several teachers of the Department of Physical- Chemistry, the handling of the simulator was simplified to provide for its use as a didactic resource for effective teaching.

At the end of the teaching period, practical laboratory simulations were evaluated by asking (anonymously) several questions to the students who had worked with the simulator the last academic year (specifically, 87 pupils), to gather information about the tasks where they found the greater difficulties.

Table 3 gives the responses of students to different aspects of the design and handling of the system. They evaluated the calculation required to obtain the appropriate flows as complicated, the menus of the program as easy to understand and the handling of the equipment as suitable for

Table 3
Answers given by the students of the last year (87 pupils) on various aspects of the simulation and the OLE Program

Calculations of the appropriate flows are	
Simple	5
Complicated	72
Very difficult	10
Menus are	
Easy to understand	79
Accessible	8
Complicated	0
Handling of the equipment	
Is not suitable for university level	2
Is suitable for university level	77
Needs a significant improvement	8

higher level education. The majority of them considered the tasks interesting and motivating. As a result, we believe that use of the simulator as a didactic tool motivates the pupils, and develops their scientific intuition and enthusiasm for discovery.

4. Final remarks

Simulations are becoming an integral part of management and engineering education as students learn by using and building simulations of complex systems and processes (Cañizares, 1997; Nahvi, 1997). As Parush et al. (2002) reported, simulations can incorporate special teaching and learning mechanisms to support the individual learner. In contrast to the real world, which is being simulated to various degrees of fidelity, the students using a simulator are able ‘‘to stop the world’’ and ‘‘step outside’’ of the simulated process to review and understand it better.

Therefore, the device constructed allows the simulation in a realistic manner of the chemical reactivity of any substance passing through an estuary, constituting a useful teaching tool that avoids many of the logistical problems involved with in situ surveys. Also students can compare their laboratory results with those obtained in the natural environment.

The OLE program appears to be a very useful tool, which has been evaluated positively by the students themselves.

It is quite feasible to apply the simulator to teach the behaviour of different substances, particularly pollutants; these only need to be introduced to the river water or to whichever of the tanks that represents the specific zone of the estuary involved. Therefore, this simulator will also be useful for carrying out a priori environmental risk assessments.

In addition to the employment of the simulator for teaching purposes, the system has also been utilised in research work by some of the researchers of the Physical Chemistry Department of the Marine and Environmental Sciences Faculty of Cádiz University (e.g., in García-Luque, Forja, DelValls, & Gómez-Parra, 2003).

References

Bale, A. J., & Morris, A. W. (1981). Laboratory simulation of chemical processes induced by estuarine mixing: The behaviour of iron and phosphate in estuaries. *Estuarine Coastal and Shelf Science, 13*, 1–10.

Burton, J. D. (1976). Basic properties and processes in estuarine chemistry. In J. D. Burton & P. S. Liss (Eds.), *Estuarine chemistry*. London: Academic Press.

Cañizares, C. A. (1997). Advantages and disadvantages of using various computer tools in electrical engineering courses. *IEEE Transactions on Education, 40*(3), 166–171.

Davies, C. H. J. (2002). Student engagement with simulations: A case study. *Computers & Education, 39*, 271–282.

Frankignoulle, M., Abril, G., Borges, A., Bourge, I., Canon, C., Delille, B., Libert, E., & Théate, J.-M. (1998). Carbon dioxide emissions from European estuaries. *Science, 282*, 434–436.

García-Luque, E., Forja, J. M., DelValls, T. A., & Gómez-Parra, A. (2003). The behaviour of heavy metals from the Guadalquivir estuary after the Aznalcóllar mining spill: Field and laboratory surveys. *Environmental Monitoring and Assessment, 83*, 71–88.

Gómez-Parra, A., DelVAlls, T. A., Forja, J. M., Sáenz, I., & Riba, I. (2000). Early contamination by heavy metals of the Guadalquivir estuary after the Aznalcóllar mining spill (SW Spain). *Marine Pollution Bulletin, 40*(12), 1115–1123.

Grasshoff, K., Ehrhard, M., & Kremling, K. (1983). *Methods of seawater analysis*. R.F.A.: Verlag Chemie.
Kearsley, G., & Shneiderman, B. (1998). Engagement theory: A framework for technology-based teaching and earning. *Educational Technology, 38*(5), 20–23.
Lebo, M. E., Sharp, J. H., & Cifuentes, L. A. (1994). Contribution of river phosphate variations to apparent reactivity estimated from phosphate-salinity diagrams. *Estuarine Coastal and Shelf Science, 39*, 583–594.
Morris, A. W. (1985). Estuarine chemistry and general survey strategy. In P. C. Head (Ed.), *Practical estuarine chemistry (A handbook)*. Cambridge: Cambridge University Press.
Nahvi, M. (1997). Dynamics of student–computer interaction in a simulation environment: Reflections on curricular issues. In *Proceedings of the frontiers in education '97*. IEEE.
Ortega, T., Forja, J. M., & Gómez-Parra, A. (2001). Teaching estuarine chemical processes by laboratory simulation. *Journal of Chemical Education, 78*, 771–774.
Parush, A., Hamm, H., & Shtub, A. (2002). Learning histories in simulation-based teaching: The effects on self-learning and transfer. *Computers & Education, 39*, 319–332.
Smith, R. E., Peterson, D. H., Hager, S. W., Harmon, D. D., Schemel, L. E., & Herndon, R. E. (1985). Seasonal and interannual nutrient variability in Northen San Francisco Bay. In A. C. Sigleo & A. Hattori (Eds.), *Marine and estuarine geochemistry*. Chelsea, MI: Lewis Publisher Inc.
St. Clair, D. W. (1989). *Controller tuning and control loop performance*. Newark: Straight-line Control Co.
Wood, T. M., Baptista, A. M., Kubawara, J. S., & Flegal, A. R. (1995). Diagnostic modeling of trace metal partitioning in south San Francisco Bay. *Limnology and Oceanography, 40*(2), 345–358.