

sented a poster about the applicability of ESI-IMS to analyze aqueous samples containing chemical weapon agents and their degradation products. The ESI-IMS system is supposed to be portable and may be utilized not only for detection of warfare agents, but also for monitoring of water supplies for safe use such as drinking water.

### Rapid Separation of Illicit Drugs by Electrospray Ion Mobility Spectrometry/Mass Spectrometry IMS/MS

Laura Markowski from Hill's group presented recent results from the group's

new home-built high-resolution IMS/MS instrument which now enables IMS to be utilized as a rapid separation device for complex mixtures. She mentioned that although ion mobility spectrometry (IMS) has been widely employed as a field-monitoring device for illicit drug detection, it has been limited to field applications due to the low resolution of commercial instruments. The group has demonstrated the rapid separation of illicit and therapeutic drugs (benzodiazepines, opiates, barbiturates, and amphetamines) by IMS/MS. The effects of complex mixtures did not affect sensitivity and selectivity significantly, possibly due to the nature of the ESI method that has an excess of charges to ionize the an-

alytes efficiently. The ESI-IMS/MS instrument can be seen on <http://www.wsu.edu/~hillh/esiimsms.html>.

The Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy is an annual event and the next meeting is scheduled for March 4–9, 2001, New Orleans. A specific meeting on IMS has been organized by the International Society for Ion Mobility Spectrometry in August 13–17, 2000, Halifax, Canada. The latter one may be of interest for those who want to get some first hands-on experience in this field.

Henrik Ørsnes

Received: March 6, 2000

# FH – HES

Fachhochschulen – Hautes Ecoles Spécialisées

Chimia 54 (2000) 370–372  
© Neue Schweizerische Chemische Gesellschaft  
ISSN 0009–4293

## Computational Chemistry for Kids

Olivier Naef\*

**Abstract:** This article aims to show that computational chemistry is not exclusively restricted to molecular energy and structure calculations but also includes chemical process control and reaction simulation. By having fun with LEGO and a fundamental knowledge of LabVIEW, it is shown how a novice can be introduced to this exciting and challenging field of chemistry.

**Keywords:** Automation · Computational chemistry · Kids · LEGO

### 1. Introduction

Computational chemistry is exotic for many people. Chemists often think that computational chemistry is restricted to

the calculation of molecular energies and geometries.

However, computational chemistry is not limited to this definition. Every chemical process that is associated with the computer, such as the control and the optimization of industrial chemical reactions, is included in computational chemistry. We can say chemical automation, but to do an online optimization of a chemical process, we need to understand not only the automation part but also the kinetics of the reaction as well as the mass and energy balance. Fig. 1 explains

the set-up of the computational chemistry study course at the University of Applied Sciences for Architecture and Technology of Fribourg (EIA-FR).

To help students or children to understand computational chemistry, the best way is to use LEGO. With LEGO, you can build a true reactor to make a simple chemical process like the dilution of a syrup. This process is interesting, because you can use ice cubes of syrup and you can automatically cool the drink. Fig. 2 gives the R&I scheme (resource and instrumentation) of this reactor.

\*Correspondence: Prof. O. Naef  
Computational Chemistry  
Department of Chemistry  
University of Applied Sciences for  
Architecture and Technology of Fribourg  
Bvd Pérolles 80  
CH–1705 Fribourg  
Tel.: +41 26 429 66 11  
Fax: +41 26 429 66 00  
E-Mail: [olivier.naef@eif.ch](mailto:olivier.naef@eif.ch)  
<http://www.eif.ch/chimie>

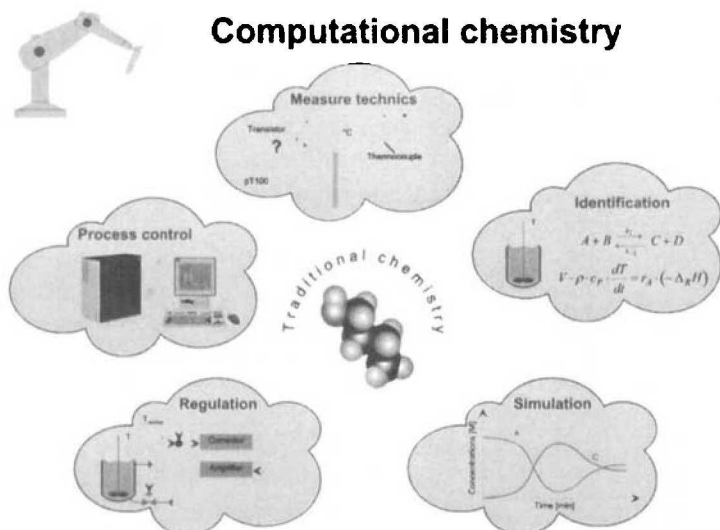


Fig. 1: Modern computational chemistry or computational chemistry for engineering

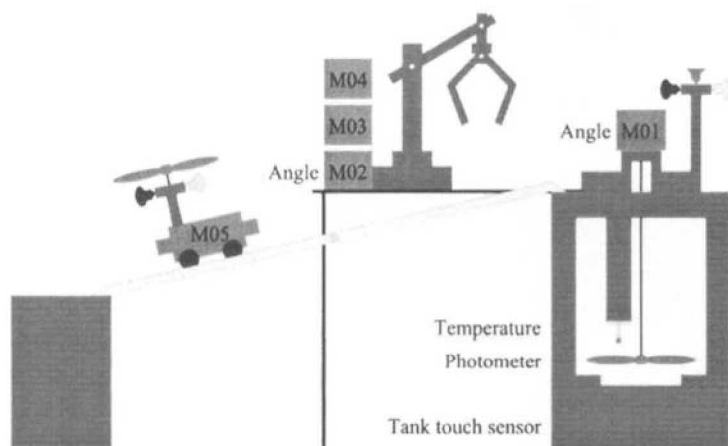


Fig. 2: R&I scheme

## 2. Lego

### 2.1. Generality

LEGO (Billund, DK), National Instruments (Texas, US) and Tufts University (Massachusetts, US) have created special technical LEGO that can be interfaced with the computer and the graphical programming language (the G language) from National Instruments (NI). The use of standard LEGO is an important step in the creativity and in the development of children. By adding computer, sensors and actuators, this world of creativity is increased. The child learns the basics of fundamental programming and the possibility to connect computers with the real world.

We have two kinds of interfaces:

- ROBOLAB, an independent system
- INTERFACE BOX called IB or LEGO engineering

### 2.2. ROBOLAB

ROBOLAB or the programmable LEGO brick (RCX) works as an auton-

omous microcomputer. It contains a microcontroller (Hitachi) with a built-in speaker. Fig. 3 shows the RCX with its docking station. The RCX has three inputs and three outputs (digital or analog).

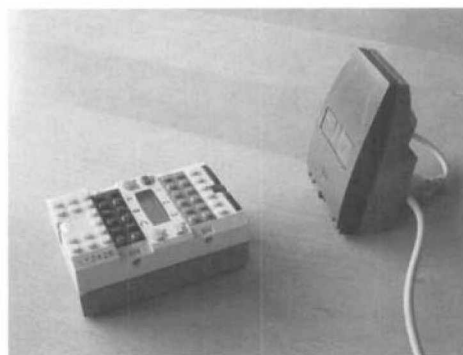


Fig. 3: ROBOLAB or the elementary brick

### 2.3. Interface Box

Fig. 4 illustrates the interface box (IB), that is capable of controlling eight input devices (sensors) and eight output devices (actuators). The IB is linked to the computer over an serial cable

(RS232). The protocol between the IB and the computer was developed by LEGO.

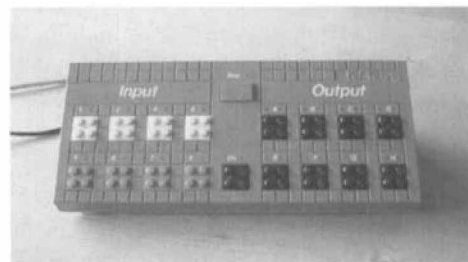


Fig. 4: The interface box (IB)

### 2.4. Sensors and Actuators

Without sensors or actuators, you cannot modify the real world. Fig. 5 shows the four LEGO sensors (temperature sensor, touch sensor, light sensor and angle sensor). Actuators are lamps, motors and sound elements. Because ROBOLAB or the IB have normalized inputs (0–5 V) and outputs (0–9 V), you can use other sensors or actuators. All these devices are completed with pneumatic systems.



Fig. 5: LEGO sensors (temperature, touch, light and angle)

### 2.5. Addresses

Ecole d'ingénieurs et d'architectes de Fribourg (EIA-FR), Département de chimie, Boulevard de Pérolles 80, CH-1705 Fribourg (<http://www.eif.ch/chimie>)

National Instruments Schweiz, Sonnenbergstrasse 53, 5408 Ennetbaden  
Tel.: + 49 56 200 5151,  
Fax: +49 56 200 5155,  
<http://www.ni.com>,  
E-Mail: ni.switzerland@ni.com.

LEGO: <http://www.lego.com>.

ROBOLAB or IB:  
<http://ldaps.ivv.nasa.gov/>.

## 3. The Installation

The installation is divided into three parts: the reactor, the crane and the transport vehicle.

### 3.1. The Reactor

The reactor is made up of a transparent plastic food container. It is surrounded by standard LEGO. A touch sensor indicates if the container is at the correct

position. A light sensor measures the intensity of the light in the reactor (a low-cost photometer). At the top of the reactor, we find an stirrer and a temperature sensor. Fig. 6 shows the reactor and Fig. 7 shows the same reactor with its opened cover lid.

### 3.2. The Crane

The crane transports the ice cubes of syrup from the transport vehicle to the reactor (Fig. 8). This crane has two axes. The rotation of the main axis uses a motor. The second axis is pneumatic and we move the crane manually. To move the pliers, we use another pneumatic system with an electro-valve (three states).

### 3.3. The Transport Vehicle

The last element is the transport vehicle. It transports the ice cubes of syrup to the crane. The entire installation is shown in Fig. 9.

### 4. Connection to the Computer

To use the IB with LabVIEW, we program a server that controls the link between the IB and the computer. This server uses two independent 'while' loops (one to receive the input samples and another one to send the commands and to maintain the communication). Fig. 10 shows the main diagram of this server.

With this server you can connect the installation to LabVIEW. Many programs can be used to control this installation. Fig. 11 gives an example of the front panel.

### 5. Conclusion

LabVIEW is a very interesting programming language for children or for people who have no knowledge in programming. The graphical programming with objects is easier to understand. To our surprise, even adult students enjoy computational chemistry by building reactors with LEGO, and by using LabVIEW to simulate the temperature profile (introduction of syrup ice cube) and to measure and control the effective values with a real system.

Received: May 9, 2000

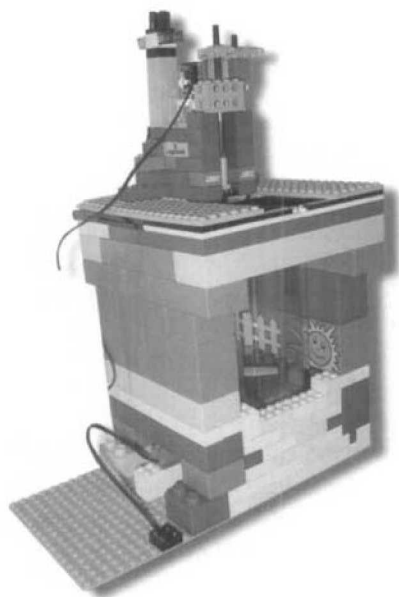


Fig. 6: The LEGO reactor

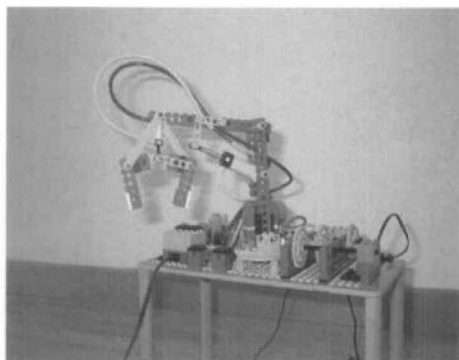


Fig. 8: The crane to transport the syrup ice cubes from the transport vehicle to the reactor

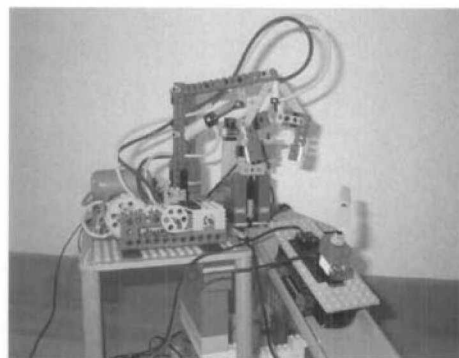


Fig. 9: Installation with the reactor, the crane and the transport vehicle

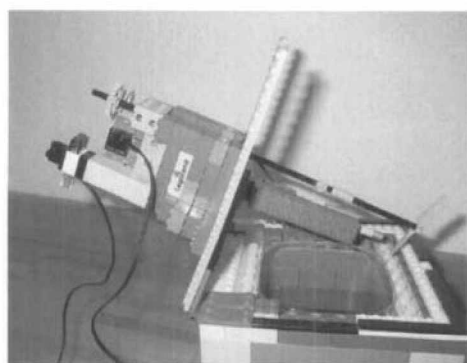


Fig. 7: The LEGO reactor with opened cover lid

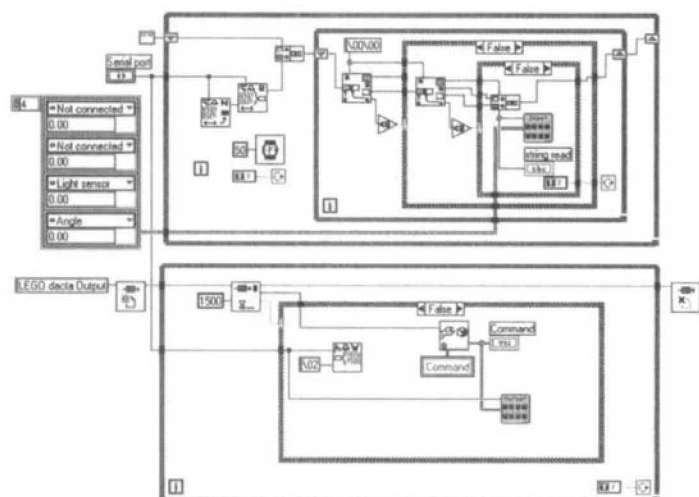


Fig. 10: Server to communicate with the interface box (IB)

### The LEGO chemical reactor

HMI - main view of the reactor

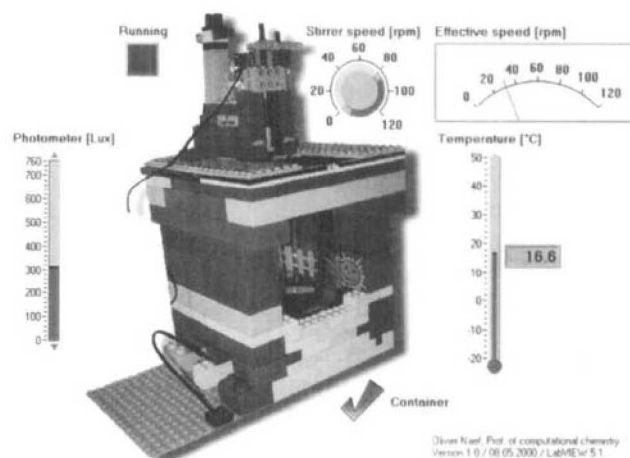


Fig. 11: Main HMI of the chemical reactor