ACTA UNIVERSITATIS LODZIENSIS
FOLIA CHIMICA 7, 1987

Zoltan M. Galbács

SIMPLE APPLICATIONS OF AUTOMATION IN CHEMISTRY

The offer refers to the application of pocket calculator and microcomputer (Sinclair - ZX-81) for conventional chemical and biochemical analytic investigations.

The presented application of the pocket calculator is based on a two--electrode indicator which counts drops, granules, colonies, gas bubbles etc.

The microcomputer of Sinclair ZX-81 has been applied to automatic treatment. The automatic burette is connected with the microcomputer and the analog-digital converter.

The whole programming is based on BASIC language.

The learning of computing forms part of the secondary school education in Hungary. Those schoolchildren who have learnt the use of computers and become university students can easily use computer techniques and apply them for an increasing number of purposes.

In the near future the use of automatic and computerized technology in all fields of economy will be a reality. Thus the industry expects the universities to produce engineers and chemists who are able to apply modern technology.

Each of the above-mentioned circumstances forces us to include automatization in university education. Unfortunately, no different automatized instruments are made in Hungary which are very suitable for chemical training. As our financial possibilities do not allow us to import, we have to construct what we need.

We may show some simple constructions. The simplicity ensures that it is easy to make numberous samples, so every student may and can use them. The demonstration of the principle of an analytical process may sometimes be more important then the result of the process. This is why the samples shown are more useful for teaching than for research chemical purposes.

A. A very simple automation can be achieved by the use of pocket calculators (which are a very common tool in chemical work; almost everybody has at least one type). A large proportion of pocket calculators can be used in the function mode, when the number entered into the register or display may be repeatedly summed by repeated pushing of the "=" key. This operation is activated by the depression of the key resulting in a closed contact between two pins of the IC, that is the resistance of the closed contact is smaller than 2-10 kohm.

If we make a terminal and the two contacts of the key are immersed into a glass of drinking water, the resistance between the immersed electrodes is low enough to activate the calculator. The increasing sum in the memory or on the display, the fluctuating light of the numbers as the electrode immersion is fluctuated, indicates that the calculator works as a counter. This phenomenon may be the basis of one type of automation.

Figure 1 shows the use of the calculator as a drop counter. The terminal electrodes are mounted onto an ion-exchange or chromatographic column. The falling drop contacts the two electrodes for a moment and activates the calculator. If we then apply number 1 to the register, the memory counts the drops of eluent.

In microbiology the number of bacterial colonies which can grow on the culture medium can be counted, as is shown in Fig. 2. One of the terminal electrodes is connected to the agar-agar salt culture medium. The other electrode is the syringe and the needle on top of it. The needle of the syringe is brought into contact with the bacteria under the control of a viewer. The conductivity of the agar-agar salt culture in the Petri dish at the moment of the touch activates the calculator.

It should be noted that in these cases the calculator is only a counter, but with no extra electronics. If we compare the prices of the pocket calculator and of the classical counter relay with its complements, it is evident why we use the calculator.

In Hungary the subsurface waters are gas- and methanebearing to such an extent that they have the potential to yield a highly inflammable and explosive mixture of gas and air [1]. On the surface, that part of the methane content which cannot be dissolved at the reduced pressure, that is at atmospheric pressure (which is

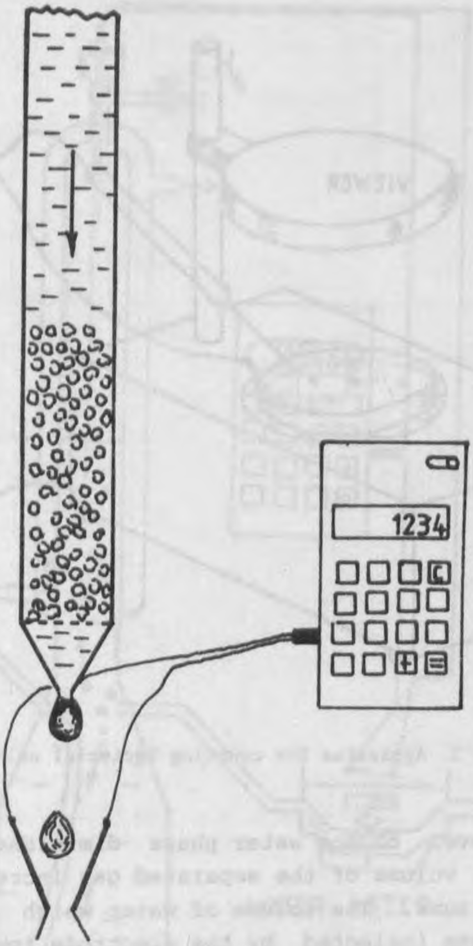

Fig. 1. Calculator as a drop counter

one-tenth or one-hundredth of the subsurface pressure), becomes free and bubbles out, and the gas and the water are separated. For gas content measurements, it is important to know the ratio of the separated gas and water volumes [2]. Figure 3 shows the collection useful for this purpose. After each water portion flow, the water meter closes the reed relay contact, which is connected in series with the calculator electrodes. The calculator sums the water meter volumes while the electrodes are immersed in the wa-

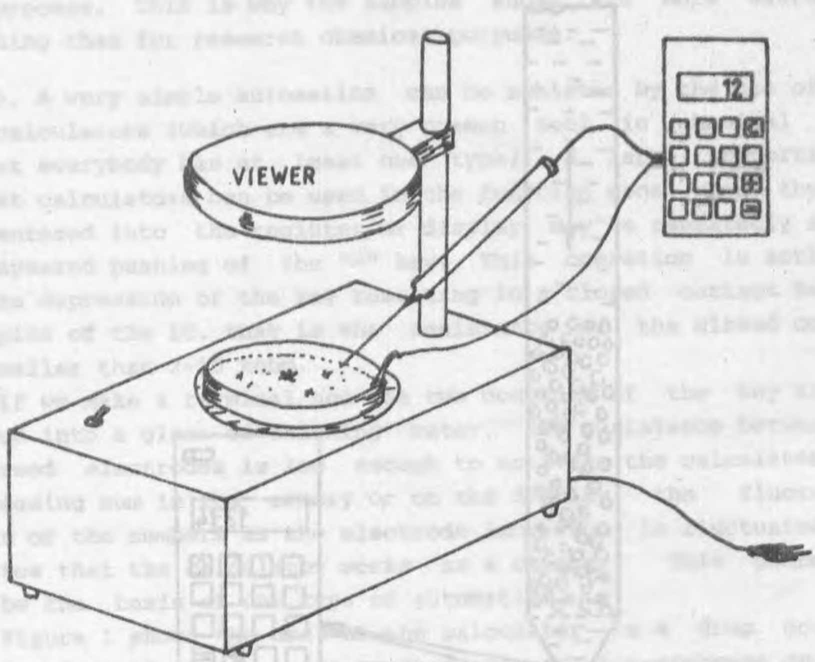

Fig. 2. Apparatus for counting bacterial colonies

ter. When the level of the water phase diminishes below the electrodes (as the volume of the separated gas increases), the calculator no longer sums. The volume of water which supplied the separated gas volume (selected by the electrode immersion death) can be seen on the display of the calculator.

The calculator can help in titrations too, as is shown in Fig. 4. The volume of the drop of titrant (or the quantity measured by it) is keyed into the register of the calculator. From this time, this value will be summed up to the end-point of the titration. The end-point can be detected by dead-stop or optical methods. In each case a very simple transistorized switching circuit closes the "clear" key, the extra terminals at the end-point of the titration. The advantage of this type of titration is that in can directly illustrate the automation, but its disadvantage is the reduced accuracy of the drop value.

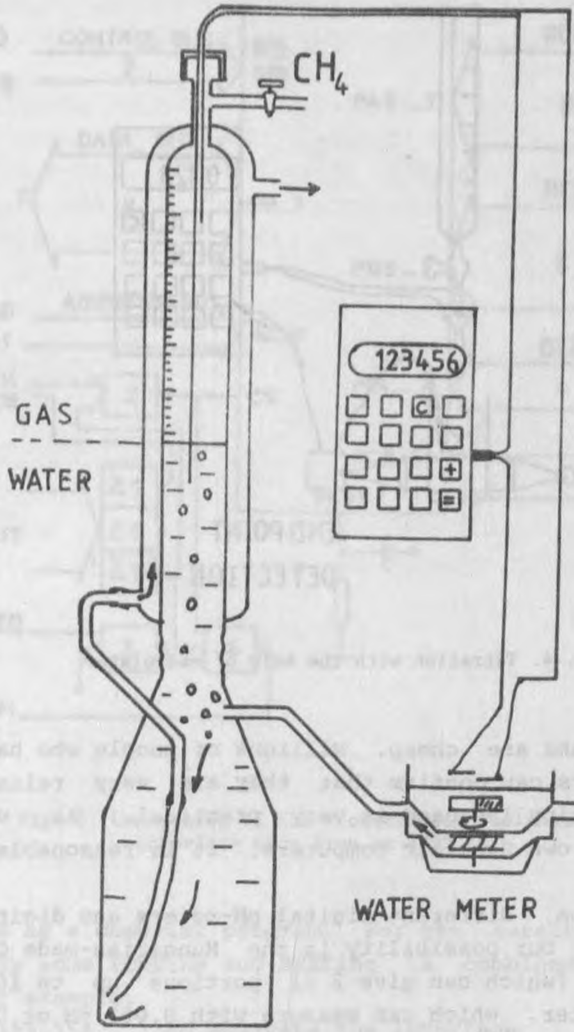

Fig. 3. Collection for the measurement of the ratio of the separated gas and water volumes

B. Real automation can be achieved with a computer connected to digital instruments. For this purpose all types of microcomputers or personal computers are suitable. However, the best choice is the Sinclair (ZX-81, Spectrum, etc.). Sinclair computers are

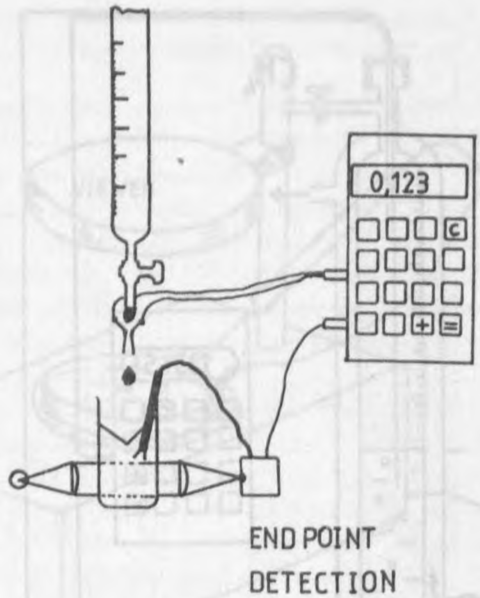

Fig. 4. Titration with the help of calculator

used world-wide and are cheap. Millions of people who have bought Sinclair computers can confirm that they are very reliable, and the BASIC programing language is very practical. As university students mainly own Sinclair computers, it is reasonable to adopt this make.

For automation, different digital pH-meters and digital burettes can be used. Our possibility is the Hungarian-made OP-930 automatic burette (which can give 2 μl portions up to 10 ml) and the OP-208 pH-meter, which can measure with 0.001 pH or 0.1 mV accuracy.

For the connection of the three instruments, we had to build an interface. This was made from an 8255 IC [3, 4]. Its function scheme is shown in Fig. 5. The interface transmits the BCD output of the pH-meter to the computer, and it transmits the instruction of the computer as a TTL impulse to the burette.

Any analytical or equilibrium problem that can be solved with a titration measuring the pH or mV sign of [5, 7] any indicating electrode can be solved automatically. The whole process has to

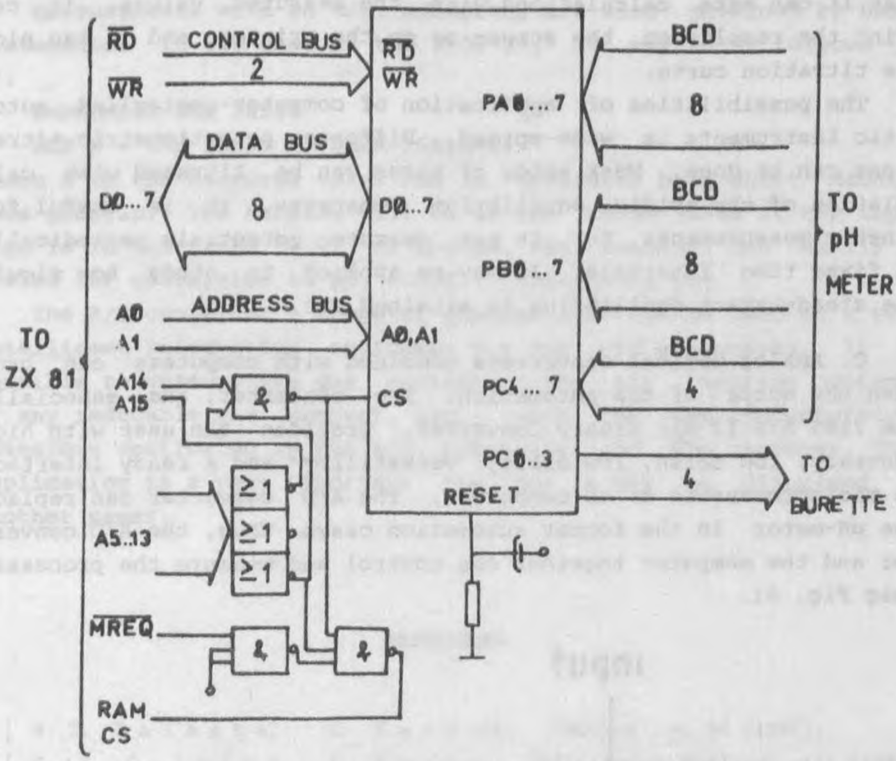

Fig. 5. Connection of the Programmable Peripheral Interface made from an 8255 IC

be presented as a computer program. For the burette and pH-meter control, only some POKEing and PEEKing is combined with the BASIC program. For example:

```
POKE 49155,154      to activate the interface
POKE 49154,2        to hold the pH-meter for reading and to step
                    the burette
PEEK 49152
PEEK 49153          to read the measured values
PEEK 49154
POKE 49154,1        to start the pH-meter (or mV measuring)
```

The use of the automatic equipment is so easy that student can write the needed program alone.

Further advantages of the use of a computer for automation is that it can make calculations with the measured values, it can print the results on the screen or on the printer, and it can plot the titration curve.

The possibilities of application of computer-controlled automatic instruments is wide-spread. Different potentiometric titrations can be done. Weak acids of bases can be titrated with calculation of the acidic equilibrium constants. It is useful for kinetic measurements, for it can measure potentials periodically at fixed time intervals. It may be applied to study how slowly the steady-state equilibrium is attained etc.

C. Analog-digital converters combined with computers can broaden the scope of the automation. The converter, and especially the 7109 A/D 12 Bit Binary Converter, provides the user with high accuracy, low noise, low drift, versatility and a ready interface to microprocessors or to computers. The A/D converter can replace the pH-meter in the former automation cases. Thus, the A/D converter and the computer together can control and measure the processes (see Fig. 6).

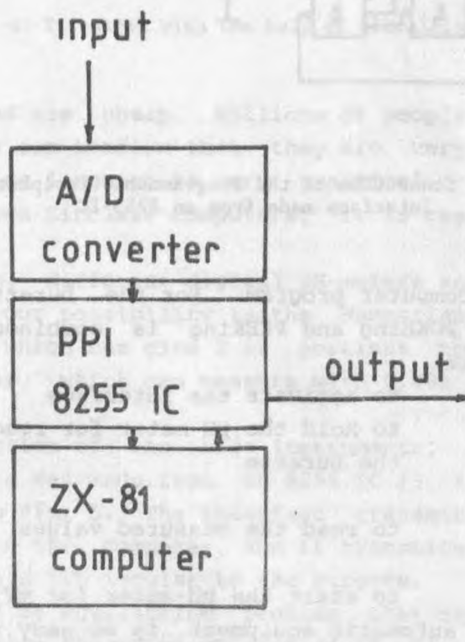

Fig. 6. A/D converter, PPI and the computer together measure and control processes

Measurements with an A/D converter are also governed by BASIC statements. In the case of the 7109 IC, it may be as follows [8, 9]:

```
RANDOMIZE USR 16520
LET X = USR 16530 x (PEEK 16515*1)
```

where X is the measured value and is generated by a short machine code program. The reading will be in the range ±4095 it the input sign is in the range ±2 V. Of course, the reading can easily be scaled for conversion to pH, e.m.f., temperature etc.

The A/D converter + computer combination can be used as a very intelligent integrating equipment for gas chromatographs. It is possible to measure the gas content in the air (methane content, or any reducable gas content, etc.) with the semiconductor-type detectors controlled by the A/D converter and the computer. This application is a very important one, but it may be discussed in another paper.

REFERENCES

[1] M. Z. G a l b á c s, I. K a s z a b, "Natura", 4, 91 (1981).

[2] M. Z. G a l b á c s, I. S e r e s, "Hidrológiai Közlöny", 411 (1981).

[3] M. P. M a c l e n a n, "Laboratory Microcomputer", 6 (1983).

[4] Gy. V a n c s ó, Elements of Microcomputers for Planning, Müszaki Könyvkiadó, Budapest 1983.

[5] M. Z. G a l b á c s, L. J. C s á n y i, Anal. Chem., 45, 1984 (1973).

[6] M. Z. G a l b á c s, L. J. C s á n y i, Magy. Kém. Folyóirat, 79, 212 (1973).

[7] K. B u r g e r, G. P e t h ö, B. N o s z á l, Anal. Chim. Acta, 118, 100 (1980).

[8] G. B u i s t, University of Surrey, personal communication.

[9] Intersil: ICL 7109 12 Bit Binary A/D Converter for Microprocessor Interfaces.

Department of Inorganic and Analytical Chemistry
University of Szeged, Hungary

Zoltan M. Galbács

PROSTE ZASTOSOWANIA AUTOMATYZACJI W CHEMII

Propozycja dotyczy zastosowania kieszonkowego kalkulatora oraz mikrokomputera (Sinclair-ZX-81) do klasycznych chemicznych i biochemicznych badań analitycznych.

Podane zastosowanie kalkulatora kieszonkowego oparte jest na dwuelektrodowym indykatorze zliczającym krople, ziarna, kolonie, pęcherzyki gazu itd.

Mikrokomputer typu Sinclair ZX-81 zastosowany został do automatycznego miareczkowania. Biureta automatyczna połączona jest z mikrokomputerem przetwornikiem analogowo-cyfrowym. Całość programowania oparta jest na języku BASIC.