

# Automated carbon dioxide measurement via miniaturised chemical reaction chambers under mechatronic control

Andrew Maxwell, Nigel Hancock, Thanh Tran-Cong  
Faculty of Engineering & Surveying  
University of Southern Queensland  
Toowoomba, Queensland, 4350, Australia  
<maxwella@usq.edu.au> <hancockn@usq.edu.au> <trancong@usq.edu.au>

## **Abstract**

*We demonstrate in this paper that by using a miniature chemical reaction vessel under adaptive mechatronic control, it is possible to design and construct a low-cost carbon dioxide measurement system which is potentially suitable for commercial application (in particular as sacrificial, single-mission instrumentation packages in horticultural cargo monitoring). Operation of the instrument is described and the need for adaptive features outlined. Performance results are illustrated and limitations noted. In addition, the results of a preliminary fluid-mechanical simulation of the reaction chamber are presented and directions for improvements noted.*

## **Keywords:**

*Mechatronic Sensing, Carbon Dioxide Measurement Turbidity Measurement, Intelligent Instrumentation.*

## **1. INTRODUCTION**

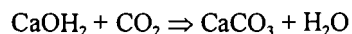
There is an ongoing requirement for low-cost gas sensing for a range of purposes including horticultural produce monitoring (for example [1], [2]) and environmental measurement (for example [3]). In these applications:

- the expected range of measurement values is known in advance, e.g. the proportion of a particular gas species in a mixture of known gasses;
- only relatively low measurement precision is required;
- logged and/or simple visual (e.g. 'out-of-range') output is required, rather than numerical displays; and
- low cost is paramount, often because the measurement system is regarded as 'single mission', i.e. is discarded after use.

One specific requirement is for the low-cost measurement of carbon dioxide produced during the transport of fresh horticultural produce, for example [2].

As set out in [4] an alternative approach for the detection of carbon dioxide (and other non-inert gasses) is via chemical reaction, and particularly those reactions in aqueous solution in which a visible precipitate is formed. The magnitude of the precipitate, and particularly its rate of development, will be directly related to the gas concentration. The developing turbidity in a previously transparent fluid may be monitored using low-cost solid-state optical components.

In the present case of carbon dioxide, the 'limewater' reaction:



provides a clearly visible precipitate ( $\text{CaCO}_3$ ).

## 2. MECHATRONIC IMPLEMENTATION

### 2.1 Basic Operation

In this instrument an embedded microcontroller (Motorola MC68HC11) provides:

- (i) control of the reaction chamber operation;
- (ii) data acquisition from the turbidity sensing;
- (iii) calculation of the carbon dioxide concentration; and
- (iv) adaptive control of the turbidity measurement process (section 2.2 below).

The basic instrumentation package comprises pumps, flowmeter, reaction cell and infra-red optics for turbidity measurement, pipelines and electronics. This package, illustrated in Figure 1, currently occupies roughly 20cm cube and is capable of considerable further miniaturisation. When provided with 1L of reagent, the instrumentation package will make and log 200 measurements of carbon dioxide concentration. With the required 1L cleaning solution, 2L waste receiver and battery power supply, the package will occupy less than 30cm cube.

Four pumps are used in the system, three for fluid pumping and the fourth for gas delivery. Chemical reagent (calcium hydroxide solution, 1.7 molar) and cleaning solution are supplied via two miniature positive displacement pumps (MFA Gear Pump, Part No 650, approximately 20mL/s) under microcontroller control. A third identical gear pump is used for draining, with a fourth pump (gas pump) and a microbridge mass airflow flowmeter (Honeywell AWM3100V) used to provide gas flow to the cell at a constant volumetric flow rate.

Maxwell & Hancock [4] set out the turbidity measurement method using infra-red optics and a microcontroller-embedded 'time-to threshold' calibration model.

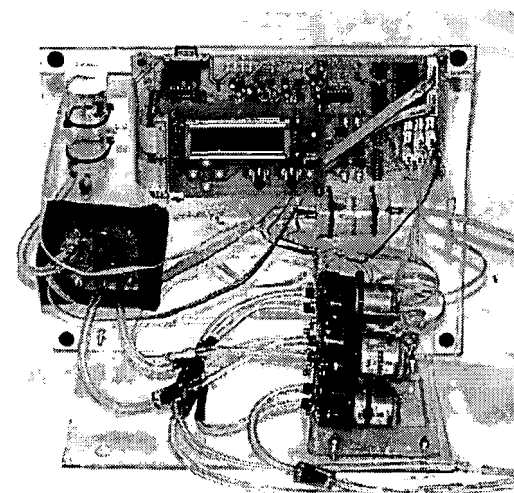


Figure 1. The prototype instrument complete except for fluid containers.

### 2.2 Adaptation to Changing Measurand Values and Measurement Conditions

Recent work has revealed that the basic operation set out above is inadequate under certain measurement conditions, in particular when the proportion of  $\text{CO}_2$  was small (<10%) and when the cell had 'aged', after performing typically 100 measurement cycles. However the intended applications of the instrument comprise sequential measurements on a single, slowly-changing  $\text{CO}_2$  source. Hence adaptation of the measurement system may be undertaken, with changes determined by prior measurements [5, 6].

Four parameters of the process have been made adjustable under adaptive control to extend the range of useful operation and maintain measurement discrimination. These are:

1. the provision of alternative baseline-to-threshold intervals (to reduce 'time-to-threshold' values);
2. the output power of the infra-red emitter -- reduced with low levels of turbidity to avoid saturation of the infra-red detector;
3. the input sensitivity for the infra-red detector -- increased for low levels of turbidity to increase discrimination; and
4. analogue gain applied to the infra-red detector signal -- to maintain discrimination at the analogue-to-digital converter.

### 2.3 Performance

Figure 2 illustrates the performance of the current prototype (using the empirically-designed reaction chamber -- see below).

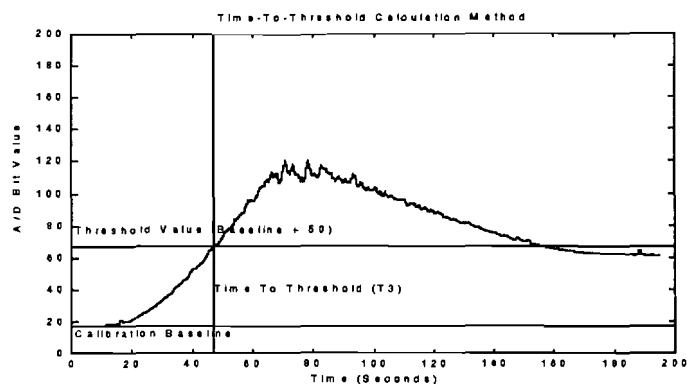


Figure 2. Attenuation development for 50%CO<sub>2</sub>, 50%N<sub>2</sub>, in terms of the output of the embedded analogue-to-digital (A/D) converter (in arbitrary units). A threshold of 'baseline + 50' is shown.

### 3. REACTION CHAMBER DESIGN

#### 3.1 Empirical Cell Design

The reaction vessel ('cell') of approximate internal volume 2.5 mL was created by milling and polishing void spaces in two 50mm x 50mm x 5mm acrylic plates and clamping them together with a neoprene gasket, as illustrated in Figure 3(a). Two printed circuit boards clamped either side of the cell (Figure 3(a)) carry an infra-red LED source (OPTEK OP165) and detector (Three-Five Systems TDET500) respectively. These are aligned to 'look through' the cell in the region of minimum of bubble activity, the 'measurement zone' indicated in Figure 3(b).

The shape of the void space and placement of ports was determined empirically [5] and includes a central 'pillar' (Figure 3(b)) to establish flow circulation. The design is a compromise between:

- maximum mixing (and hence development of precipitate);
- the provision of an adequately 'quiet' bubble-free measurement zone;
- the entrapment of gas for exhaust without loss of reagent; and
- cleanability, i.e. the effective removal of precipitate with a minimum quantity of cleaning fluid.

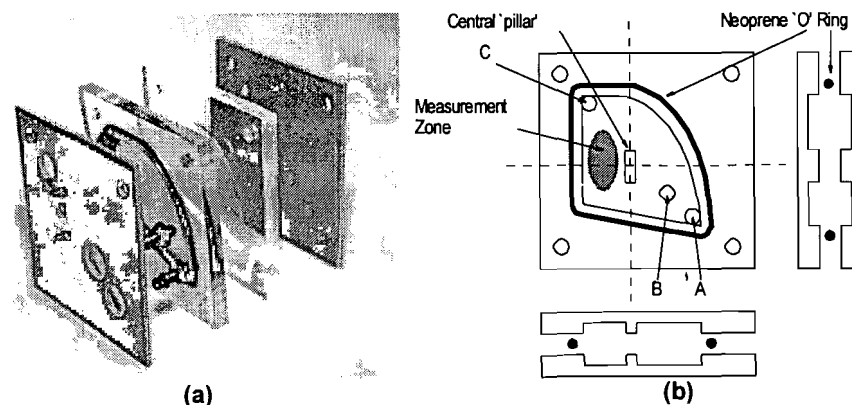


Figure 3. The 'teardrop'-shaped chemical reaction cell. (a) Cell plus infra-red optics circuit boards disassembled but in its operational (vertical) orientation. (b) Cell construction showing the three ports, A, reagent entry, exit and flushing; B, gas entry and C, gas exhaust; the measurement zone, indicated and the central 'pillar' which encourages flow circulation.

Figure 4 shows the cell containing reagent and gas under operational conditions. An additional pair of infra-red source and detector are used to establish the fluid level shown in the figure. Gas bubbling through the cell displaces air in the upper corner escapes via the exhaust port of the cell (Figure 3 – 'Port C'). Obviously, a vertical orientation must be maintained during operation.

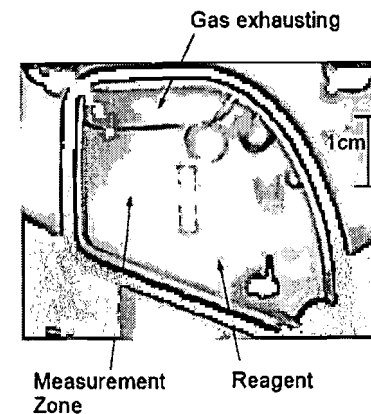


Figure 4. The measurement cell under operational conditions (video capture).

#### 3.2 Cell Analysis and Discussion

In order to improve the cell design, and hopefully permit further miniaturisation, an understanding of the flow dynamics of the cell is required. As previously

mentioned, an optimal cell will maximise mixing, encourage bubble-free measurements, permit efficient gas exhausting, and have easy cleaning properties. Some of these properties are related to the internal design of the cell milling shape, and the placement of the ports, hence it was seen advantageous to perform some analysis of the ‘tear-drop’ cell shape, in order to assist in the design of future cells.

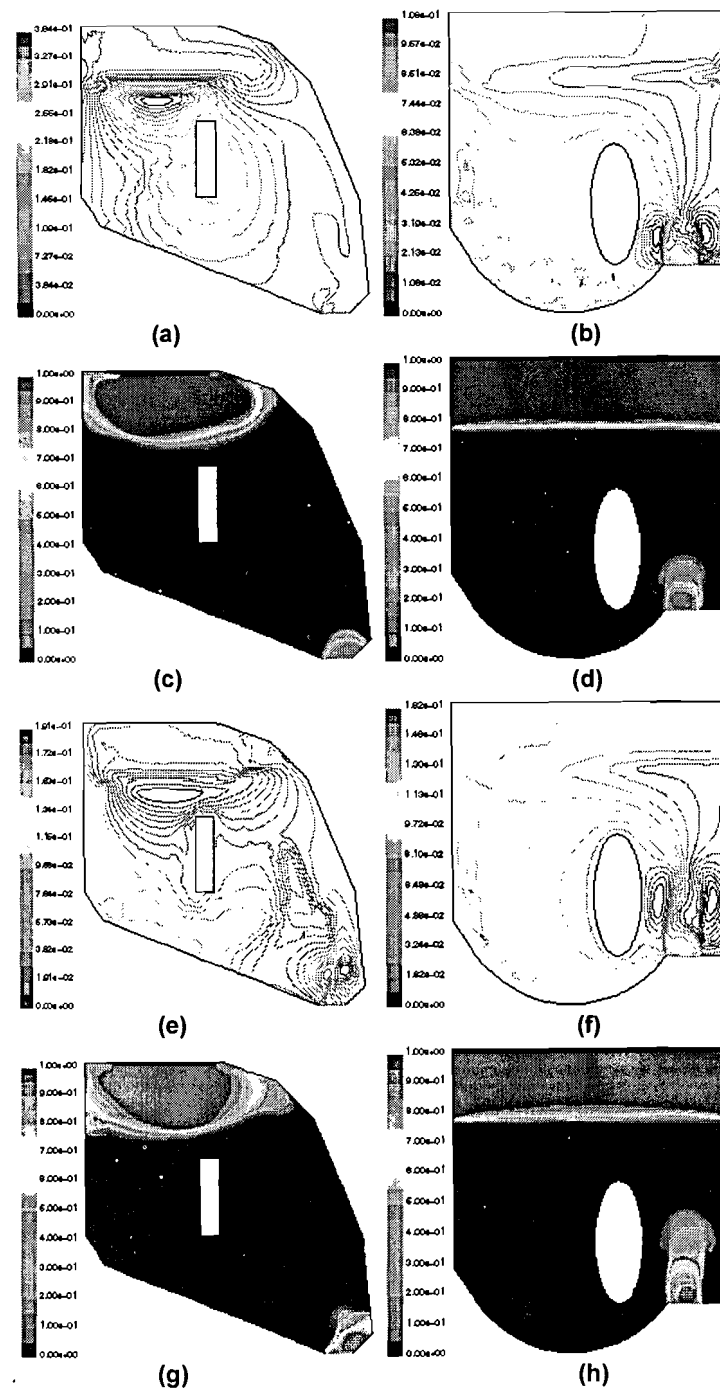
Clearly the present problem is very complicated due to the complex transient interaction between chemical reaction, mass transfer and fluid dynamics, not to mention heat transfer. The range of parameters that can be optimised is extensive which makes the experimental trial-and-error approach impractical. Modern numerical methods can offer a means for optimisation of the cell design. As a first step towards that goal the fluid dynamics problem is attempted here in order to gain insight into the flow patterns associated with particular geometries.

The Computational Fluid Dynamics software ‘Fluent’ is used to simulate the flow in two cells: firstly using the geometry of the existing experimental cell (Figures 3 and 4) and secondly one arbitrarily chosen with a narrower channel for the rising bubble (refer Figure 5, right hand side). The gas inlet is similarly located at the bottom right corner and the vent is at the upper left corner of the cell.

Figure 5 illustrates the simulation results for both geometries. The flow patterns and the gas-liquid interfaces are shown at 0.1s and 0.2s from the start of the gas injection according to the arrangement of Table 1. The streamfunction plot for the experimental cell shows that high shear rate flow regime develops near the upper left region in contrast with the flow pattern in the other cell where high shear rate flow regime develops next to gas bubble. Of course such a high shear rate flow regime next to the bubble is highly desirable from the point of view of facilitating the chemical reaction. Although these are very preliminary results they serve to illustrate the direction of our future investigation.

**Table 1. Layout and simulation conditions for the eight results shown in Figure 5. The vertical greyscale in each indicates:**  
 (a),(b),(e),(f) – low (bottom) to high (top) value of the stream function (arbitrary units).  
 (c),(d),(g),(h) – liquid (bottom) to gas (top) phase (for which the expected step change liquid-to-gas is not modelled by the software).

Experimental Cell	‘Alternative’ Cell
(a) 0.1s Stream Function	(b) 0.1s Stream Function
(c) 0.1s Phase Plot	(d) 0.1s Phase Plot
(e) 0.2s Stream Function	(f) 0.2s Stream Function
(g) 0.2s Phase Plot	(h) 0.2s Phase Plot



**Figure 5. Analysis of the fluid and bubble flow – refer Table 1.**

#### 4. CONCLUSION

The authors suggest that the feasibility of a miniaturised and fully automated 'wet chemical' approach to carbon dioxide gas measurement has been demonstrated. The potential utility of the approach in measurement situations requiring a disposable (single mission) system has been argued.

Significant shortcomings and limitations principally due to modest components deliberately-chosen for their low cost, have been largely overcome by adaptive techniques embedded in software.

Fluid-mechanical simulation of the cell, although very preliminary, indicates that the empirically-designed cell geometries may be significantly improved. In turn this promises reduced measurement times and further miniaturisation, hence reduced reagent requirements and reduced overall size of the instrument.

#### ACKNOWLEDGEMENT

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