TOF Operating modes

The overall Time Of Flight (TOF) system can be operated in several different modes depending on the experimental requirements. These can be summarised as follows:

Note: In the following description, references to laser fire are to indicate when the laser would be triggered. No laser experiments are reported in this work.

Beam on only

The pulse beam and the laser fire every time. Figure 3.1. The TOF unit adds the data to the same spectrum every time. This mode is only suitable in high-signal and low-noise situations.

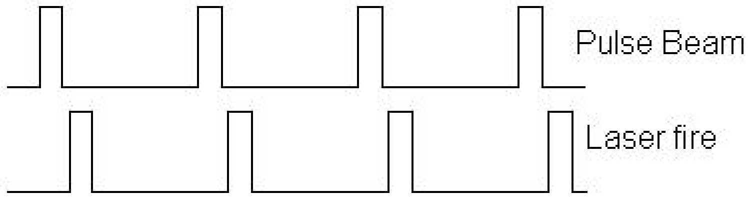

Figure 3.1 Beam On only

Alternate beam on only

The pulse beam fires every second time and the laser fires every time. Figure 3.2 It allows molecular beam-on / molecular beam-off spectra to be accumulated separately for background subtraction.

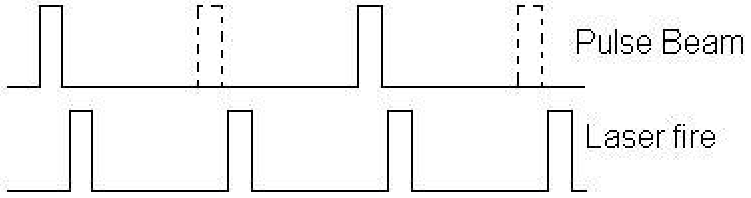

Figure 3.2 Alternate beam only

Alternate mode

The pulse beam fires every time and the laser fires every second time. Figure 3.3 This is used for laser-on/laser-off experiments. The TOF puts the data into two different spectra for the two laser signals. Subtracting one from the other removes background from non-laser signals. Subtracting one from the other removes background from non-laser sources.

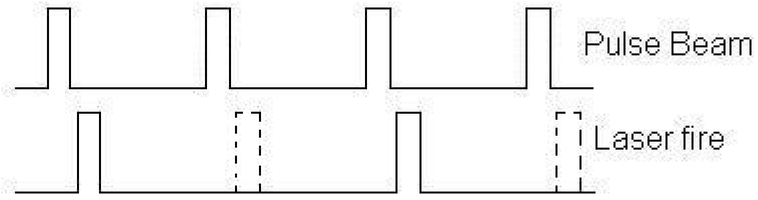

Figure 3.3 Alternate mode

TOF electronics

The Time Of Flight (TOF) electronics are responsible for synchronising the different active elements of the overall system and acquiring ion counts from the detector. In practice, the system is based around two custom built controllers: the TOF timing unit and the TOF data acquisition unit. These controllers were originally operated remotely by an Apple Macintosh via a RS232 and IEEE control bus respectively.

The TOF acquisition controller has been replaced by a custom build PC-card based dual channel ion counting system. This has hardware and software fast ion counting circuitry controlled by a dedicated PC. This PC also handles communication with the TOF timing unit.

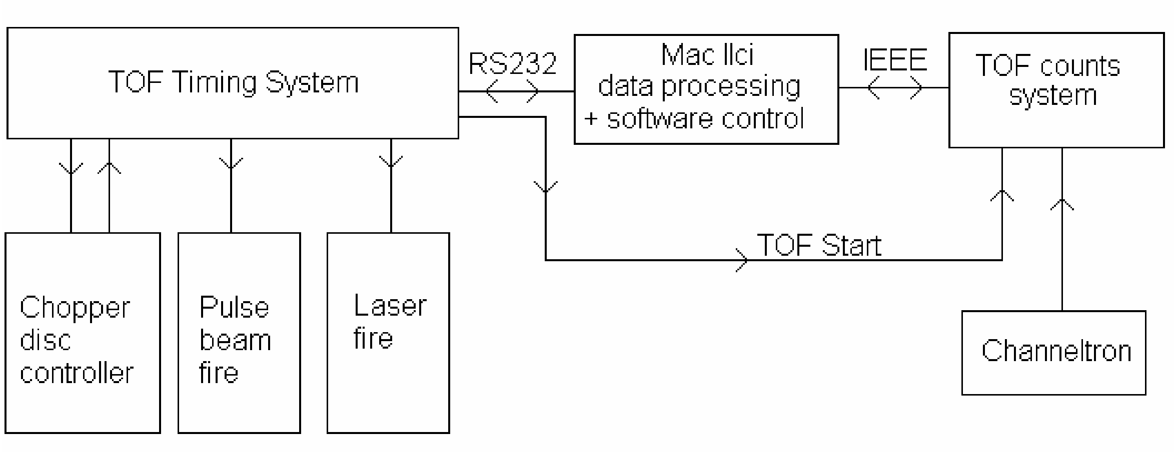

Figure 3.4 Old system schematic

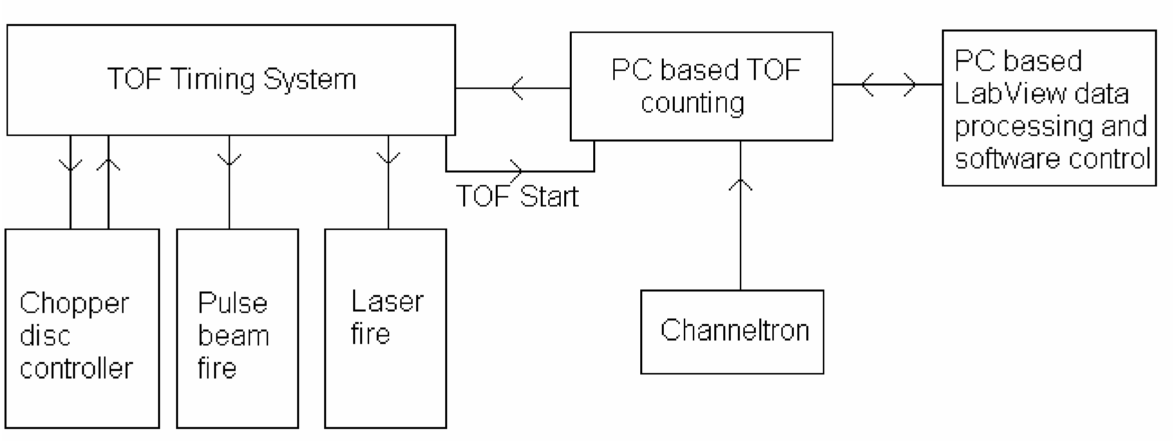

Figure 3.5 New system schematic

TOF timing unit

The TOF timing unit provides the central synchronised timing pulses for the pulse beam, the dual scalars, the laser (if required) and to trigger the TOF data acquisition unit. The timing unit also controls the rotational speed of the slotted disc. Running parameters can be entered via a keypad or RS232 link.

PORTS:

Chopper disc reference: receives TTL pulses from the rotating chopper disc to indicate slot position

Beam On•: indicates Beam ON cycle is active

Beam Off•: indicates Beam OFF cycle is active

Laser fire•: TTL pulse to fire

Pulse beam fire•: TTL pulse to fire pulse beam during both Beam ON and Beam OFF

Alternate pulse beam fire•: TTL pulse to fire pulse beam during Beam ON only

TOF start•: TTL pulse initiates data logging

Sine wave•: digitally generated sine wave to drive chopper motor

RS23••: 9600 baud datalink to PC

• denotes output
•• denotes bidirectional

TOF data acquisition

The actual acquisition uses a dedicated microprocessor and hardware circuitry. The basic program handles communication with the LabView PC, the acquisition card and the TOF controller.

TOF system timing

The timing sequence for a typical experiment is as shown in Figure 2.14

Time period definitions

T_p slot period	T_t TOF start delay	T_x pulse beam opening time
T_l laser fire delay	T_d pulse beam fire delay	T_f nozzle-disc flight time

Once a ‘pulse’ sequence is initiated, the TOF timing unit waits for a disc reference pulse to indicate that a slot has arrived at the beam axis. After a predetermined delay, the Pulse beam fire delay T_d, a pulse beam fire signal is generated to initiate a gas pulse. This travels from the nozzle and a portion of it passes through the successive slot. A beam start pulse is generate in synchronism with this second slot to indicate a gas pulse is leaving the pulse beam. Two other signals are initiated in parallel to this beam start pulse: a laser beam fire pulse used to trigger the laser (if required), and a TOF start pulse used to trigger the data acquisition. Both of these signals are delayed by predefined time periods, TOF start delay T_t and Laser fire delay T_l respectively. The TOF start delay is set so that data acquisition begins slightly before molecules reach the detector.

Although the pulse beam delay is optimised experimentally, the delay corresponds to:

$$T_d = T_p - (T_x + T_f + T_{hsw}) \quad (3.1)$$

The slot period T_p is given by the rotational speed of the disc and the number of slots. E.g. for an eight slotted disc rotating at 200Hz, the slot frequency = 1600Hz. The slot period is therefore 625µs. The pulse beam opening time T_x is a constant 200µs. A correction factor T_{hsw} (half the slot width time = 18µs) is added to account for the fact that system timing is synchronised with a slot edge rather than a slot centre. The nozzle disc flight time T_f is determined by the time taken for a given molecular species to traverse the 3.6cm nozzle-disc distance.

T_d = 625 – (200 + 90 + 18) = 317 µs, which is relatively close to the measured optimal figure of 295µs.

TOF time correction

Having acquired a set of experimental data, the time component must be corrected before any form of numerical processing is performed.
There are three main corrections that are made to the time channel:

a) Chopper slot width correction

The opto-sensor mounted on the chopper disc within the pulse beam assembly triggers on the edge, rather than the centre line, of a slot. To synchronise the (t=0) event with the centre of a slot (i.e. with the beam peak intensity), a correction factor is added to shift the effective start of a timing sequence. This factor is determined by the chopper disc rotation speed and the slot width.

b) Beam nozzle-surface flight time

There are two basic configurations that are available with this system:
i) Direct beam measurements, where the pulse beam is aimed directly at the detector. (Effective flight distance = 567 mm)
ii) Scattering experiments, where the pulse beam is aimed at a sample surface at one angle and the detector aligned to the surface at a second independent angle. (Surface-detector flight distance = 500 mm)
In all measurements, the (t = 0) event is initially synchronised with the firing of the pulse beam. This is appropriate for all direct beam measurements. However, when attempting to analyse surface distributions, it is important that the (t = 0) event is synchronised with the instant that the molecular beam impinges on the surface.
Thus for scattering experiments, it is necessary to remove an offset factor to account for the time taken for the gas pulse to leave the nozzle and impinge on the surface. This beam nozzle-surface flight time is given by:

$$T_{NS} = \frac{\text{Nozzle - surface distance}}{\text{Average beam velocity}} \qquad (3.2)$$

The nozzle-surface distance is a constant 67 mm. The average beam velocity of each gas mixture is obtained by performing a direct beam measurement and observing the peak of the velocity distribution. This calculation is performed automatically within the ‘main experimental parameters’ whenever the ‘Direct Beam’ option is selected.

Once a T_{NS} correction time is established, it may subtracted from the time channel of an experimental set when the data is exported from the TOFSys program. The corrected data set is the imported into a numerical analysis program TOFfit for curve fitting an evaluation.

a) Ion time

The time T associated with any particular acquired data channel is the sum of two components: the time taken to traverse from beam/surface to the centre of the ioniser (distance d_1) and the ion time, the time taken to traverse from centre of the ioniser to the detector (distance d_2).

In order to correct for the presence of the ion time in the data, and to determine the true velocity for each point, a correction procedure is used:

If we assume that an ion created in the ioniser receives an abrupt increase in translational energy E upon its extraction from the ioniser, the ion velocity is defined by:

$$\Delta E = \frac{1}{2} m\, v_i^2 \quad (3.3)$$

and the corresponding ion time is:

$$t_i = \frac{d_2}{v_i} \quad (3.4)$$

The total flight time is therefore

$$T = \frac{d_1}{v} + \frac{d_2}{\sqrt{v^2 + v_i^2}} \quad (3.5)$$

The corrected experimental time of flight t_n and its corresponding velocity v_n for a particular channel n is given by the following iterative relation [1]:

$$v_i = \frac{d_2}{t_i} \quad (3.6)$$

$$T_n = nTW + TD - TC - (0.5TW) - TU \quad (3.7)$$

$$v_n^0 = 0$$

$$t_n^{k+1} = T_n - \frac{d_2}{\sqrt{(v_n^k)^2 + (v_i)^2}} \quad (3.8)$$

$$v_n^k = \frac{d_1}{t_n^k} \quad (3.9)$$

t_n = corrected experimental time of flight for the nth channel
v_n = corrected experimental velocity for the nth channel
TW = channel width   TD = TOF delay   TU = 0.2 µs**
TC = chopper slot width correction   (18 µs for 8 slot disc @ 200Hz)
T_n = total (measured) flight time in the nth channel
k = iteration index 1-5
**- To compensate for a built in timing delay in the data acquisition unit of 200 ns

References

1) D. St. A. G. Radlein, PhD thesis, Cambridge University (1975)