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FlashPhotol: Using a Flash Photolysis Apparatus Simulator To Introduce Students to the Kinetics of Transient Species and Fast Reactions

Stephen W. Bigger*

College of Engineering and Science, Victoria University, Melbourne, Victoria 8001, Australia

Ⓢ *Supporting Information*

ABSTRACT: FlashPhotol is an educational software package that introduces students to the kinetics of transient species and fast reactions. This is achieved by means of a computer-simulated flash photolysis apparatus that comprises all major functional elements and that students can use to perform various experiments. The experimental interface presents a visual representation of the monitoring light beam transmission through the sample cell as well as the corresponding transient concentration after excitation thereby enabling students to fully appreciate the fundamental processes on which the technique relies. Experiments in the package also reinforce students' understanding of the Beer−Lambert law and illustrate how an absorbance value is produced from internal signals within an instrument. The software includes: (i) a fully contained tutorial on the technique of flash photolysis; and (ii) a procedure for each of the experiments that can be performed using the simulator along with an example results analysis in each case. It is anticipated that instructors may wish to use the simulator for lecture demonstrations, especially in demonstrating the transient process occurring in the sample cell following flash irradiation.

KEYWORDS: *Second-Year Undergraduate, Upper-Division Undergraduate, Physical Chemistry, Computer-Based Learning, Inquiry-Based/Discovery Learning, Kinetics, Photochemistry, Spectroscopy*

■ INTRODUCTION

The flash photolysis technique has been widely used to study light-induced processes in polymers, organic species, semiconductors, and nanoparticles, as well as photosynthesis in plants. The general areas of application of this technique are wide and include chemistry, biology, materials science, and environmental science. Given the wide application of this technique and its significance as reflected in the award of the 1967 Nobel Prize for Chemistry to its originators,[1,2] it is a most appropriate topic for inclusion in the chemistry curriculum.

■ SIMULATION SOFTWARE

The FlashPhotol desktop software package comprises a tutorial on the basics of the technique of flash photolysis and a flash photolysis apparatus simulator that introduces students to the kinetics of transient species and fast reactions. In particular, the software can be used to perform experiments to determine: (i) the kinetic rate constant of a fast reaction involving a transient species; and (ii) the absorption spectrum of the transient. In running the experiments, students consider the spectral response characteristics of the apparatus to gain an understanding of how the experimental conditions can be optimized to achieve the maximum instrument sensitivity. It is estimated that the exercises can take between about 30 min (brief exploration) and about 90 min to complete (more complete exploration with more measurements for higher spectral resolution, etc.) depending on the extent to which the user wishes to explore the topic.

The software is supplied with Supporting Information that includes all of the theoretical and experimental material that can be accessed from within the software. The package could be used in schools that do not have such an apparatus. It may also be of interest to instructors as a replacement for a lab-based experiment, a pre-lab exercise that precedes a flash photolysis laboratory class or a visual aid for a lecture demonstration. FlashPhotol comprises four interfaces that are accessed by appropriate tabs that appear on the screen: Theory, Experiment, FlashPhotol, and Lab Book.

Theory Interface

The Theory interface presents a scrollable window in which the basics of the technique are explained along with the educational literature associated with the topic.[3−10] The major functional elements common to nearly all flash photolysis experimental apparatuses are systematically discussed: flash tubes and excitation sources; monitoring beam sources such as xenon, deuterium, and halogen lamps; monochromators; sample cells; photomultiplier tubes; and analog-to-digital converters.

Experimental Interface

The Experiment interface contains a series of step-by-step experiments that can be performed using the simulator within the FlashPhotol interface of the software. The user can easily switch between these interfaces without interrupting the continuity of the experiment and can obtain a printed version of the experimental notes if required.

The first experiment is an exploratory exercise composed of two activities. The first is designed to familiarize the user with the controls of the simulator and the second explores the

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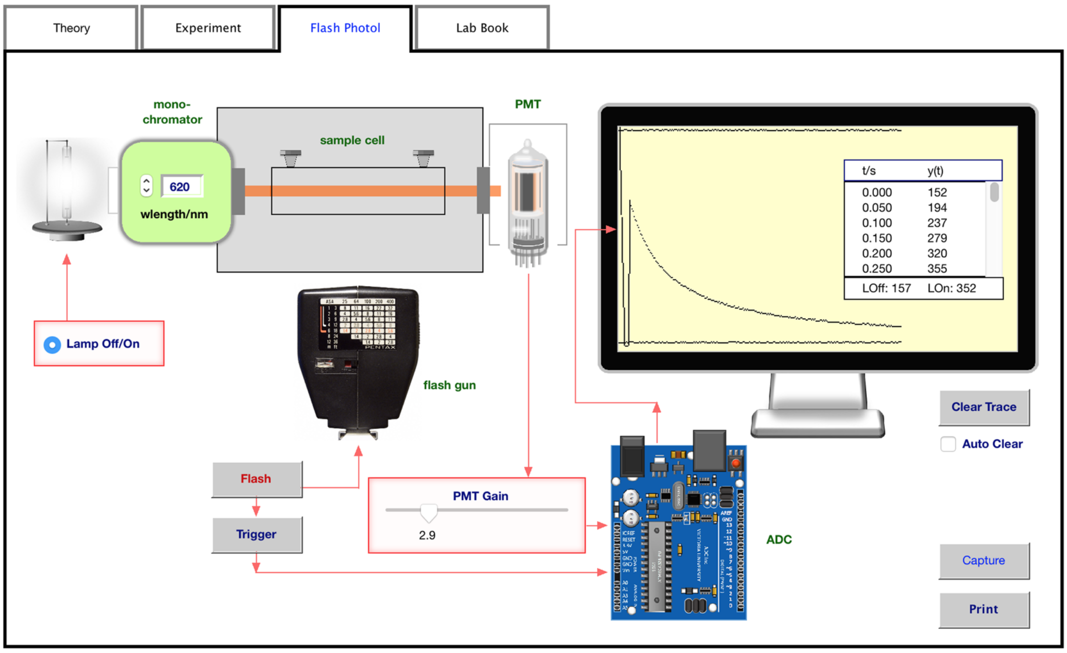

Figure 1. User interface of the FlashPhotol simulator.

instrument response characteristics. The latter provides an understanding of the combined effects of the apparatus' functional elements on its sensitivity across the spectral range of operation. Such an understanding is, in turn, needed in setting the optimum experimental conditions in the later experiments. The second experiment is the flash photolysis study of the photopinacolization of a water-soluble benzophenone derivative (4-methylsulfonate-benzophenone). The experiment is modeled on a research study in which the kinetics of the photopinacolization of this compound and the absorption spectrum of the transient species have been reported.[11] During the experiment, students acquire the raw data from the flash photolysis simulator and, in conjunction with a suitable spreadsheet program, use these data to calculate the second-order rate constant for the photopinacolization process. The obtained value is then compared with the literature value. The data acquisition and analysis are conducted at different settings of the apparatus to illustrate the importance of operating it under the conditions that produce its optimum sensitivity. The third experiment illustrates how a series of absorbance decay profiles of the transient species, obtained at different monitoring wavelengths, can be used to construct the absorption spectrum of the transient. The student also uses the absorption spectrum along with extinction coefficient information to calculate the extinction coefficient of the transient at various wavelengths and these data are compared with values given in the experimental notes.

FlashPhotol Interface

The functional elements of a flash photolysis apparatus are shown on the FlashPhotol interface (see Figure 1). The simulator has been modeled along the lines of various apparatuses described in the educational literature that have been designed specifically to illustrate to students the principles of flash photolysis.[4−8] In general, such apparatuses are usually constructed from simple components that are readily available. For example, a common photographic flash unit can be utilized as a polychromatic excitation source to produce the transient species.

The simulator shows a sample cell containing a solution that can be irradiated by a pulse of light from a commercial flash unit positioned at right angles to the sample cell. A monitoring light beam produced by a xenon arc lamp is passed through a monochromator that operates in the wavelength range of 400−750 nm and is adjustable at 1 nm increments in this range. The beam emerging from the monochromator passes through the sample cell and onto a photomultiplier tube (PMT) detector. The PMT signal (arranged to be a voltage) is passed to an analog-to-digital converter (ADC) that is interfaced to a computer. When the apparatus is triggered, the ADC samples the PMT signal at regular time intervals (0.05 s) and the generated data are displayed, along with the resulting profile on the computer screen. The data collected during each triggered event are automatically transferred to the Clipboard for ease of export to a suitable spreadsheet program for processing. The data in the Clipboard can also be filed in the form of a tab-delimited ASCII text file to be read later into a spreadsheet program if desired. An image of the simulator screen can also be printed.

Lab Book Interface

A summary of the data files is compiled in the Lab Book interface of the simulator when experimental data are captured and data files are created thereby allowing users to keep track of their data during the course of running the various experiments. The Lab Book also enables the user to access model data obtained from each of the experiments, and these data, along with their corresponding analyses, can be displayed as an instructional aid. If required, the file summary data in the Lab Book interface as well as the processed model data screens can each be printed.

FlashPhotol Versions

The FlashPhotol software comes as a stand-alone application with separate versions that run either on standard Macintosh OSX or Windows environments. A standard spreadsheet

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program for the processing, plotting and labeling of the output data should be run in conjunction with the software to provide maximum flexibility in presenting and collating the output data. The software is also supplied with associated content (i.e., theory, experiments, figures, example data and analysis) in the form of a pdf file.

OPERATING SYSTEMS

It is anticipated the software will successfully run on a wide range of Macintosh and PC systems, examples of which are given below.

Macintosh

The software has been run successfully on Macintosh computers configured as follows:

- iMac 2.66 GHz Intel Core i5; Mac OS X 10.10.5 (Yosemite); Fuji-Xerox ApeosPort-V C4475/C5575 network printer.
- iMac 4 GHz Intel Core i7; Mac OS X 10.11.4 (El Capitan); Canon MG3500 series desktop printer.
- Macbook 2.16 GHz Intel Core 2 Duo; Mac OSX 10.10.5 (Yosemite).

PC Systems

The software has been run successfully on PC computers configured as follows:

- Lenovo Thinkpad Yoga, Intel Core i7, 64-bit OS, Windows 10 Home edition; Fuji-Xerox ApeosPort-V C4475/C5575 network printer.
- Lenovo ESA4C406-86, Intel Core i5, 64-bit OS, Windows 7 Enterprise; Fuji-Xerox ApeosPort-V C4475/C5575 network printer.

CONCLUSIONS

The FlashPhotol software package is a valuable tool in teaching how the kinetics of transient species and fast reactions can be studied and quantified. The simulator enables students to observe a representation of the processes taking place in the sample cell during the transient lifetime, which in most cases cannot be directly observed in a laboratory experiment. The package also reinforces students' understanding of the Beer–Lambert law and illustrates how an absorbance value is produced from internal signals within an instrument.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00896.

All printable documentation contained within the simulator; theory notes; instructions for experiments; questions and exercises pertaining to the experiments; diagrams and information plates; typical results; derivations of equations (PDF)

FlashPhotolV3.0-Software (ZIP)

AUTHOR INFORMATION

Corresponding Author

*E-mail: stephen.bigger@vu.edu.au.

Notes

The authors declare no competing financial interest.

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