BNL-113554-2017-JA

**A software for managing chemical
processes in a multi-user laboratory**

Fernando E. Camino

Submitted to the Journal of Chemical Health and Safety

October 2016

Center for Functional Nanomaterials

Brookhaven National Laboratory

**U.S. Department of Energy
USDOE Office of Science (SC),
Basic Energy Sciences (SC-22)**

Notice: This manuscript has been authored by employees of Brookhaven Science Associates, LLC under Contract No. DE-SC0012704 with the U.S. Department of Energy. The publisher by accepting the manuscript for publication acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

A software for managing chemical processes in a multi-user laboratory

F E Camino

Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973

E-mail: fcamino@bnl.gov

Abstract. We report a software for logging chemical processes in a multi-user laboratory, which implements a work flow designed to reduce hazardous situations associated with the disposal of chemicals in incompatible waste containers. The software allows users to perform only those processes displayed in their list of authorized chemical processes and provides the location and label code of waste containers, among other useful information. The software has been used for six years in the cleanroom of the Center for Functional Nanomaterials at Brookhaven National Laboratory and has been an important factor for the excellent safety record of the Center.

1. Introduction

Multi-user laboratories, in which different chemical processes are performed, share common safety concerns. Commonly, problems arise in the following stages of work: 1) when users perform unauthorized chemical processes, and 2) when users dispose chemicals in incompatible waste containers. We have developed a software that implements a work flow aimed at reducing these potentially hazardous situations. The software allows users to perform only those chemical processes for which they have received training and authorization from staff: each user has a personal list of *authorized chemical processes*. Once a user selects a chemical process, the software gives the location and label code of the corresponding chemical waste container. In addition, the software provides other useful information, such as standard operating procedures and chemical safety data sheets.

The concept of *authorized chemical process* is of capital importance for the safety effectiveness of the software presented in this work. It consists of a chemical process with a well-defined procedure (also known as standard operating procedure or SOP), which has been evaluated by staff chemists and environmental, safety and health (ES&H) experts in order to minimize the risks that the process presents and for which safety controls have been implemented in a hierarchical order of effectivity.¹

The software was developed using LabVIEW 2014 Base System. Following a request by the authors for DOE approval, the code may be made available as open source. Similar user facilities can modify the software to fit their operations, or, alternatively, can build their own applications based on the safety concepts and structure of the software presented here.

2. Description of the software

Fig. 1 shows a diagram of the work flow implemented by the software. Before performing any chemical process, users are instructed to log on the software and select the required process from their

authorized list. *If a process is not on their list, users are instructed not to perform it.* Fig. 2 shows the software's user interface in which a user has selected a chemical process. As a result, it displays the corresponding waste container label code (A-I-2 in the example in Fig. 2). The first letter and Roman numeral in a bottle code designate the cabinet where segregated waste containers are stored. The letter corresponds to the type of waste (A for acids, B for bases, etc.) and the Roman numeral indicates the cabinet number. The MAP OF WASTE LOCATIONS button in the user interface displays a schematic blueprint of the lab with the locations of waste cabinets (see Fig. 3). The SOP and MSDS buttons display the process's standard operating procedure and the material safety data sheets of all the chemicals utilized in the selected process. The "Description/precaution" field contains a summary of the chemicals used, the hazards and the controls implemented for the procedure. An expanded version of this information is encountered in the SOP document, which can be accessed with the SOP command (Fig. 2).

Figure 1. Flow diagram of the work flow implemented by the software.

waste-log-v4.vi

Cleanroom Chemical Process Log Station

Life number: 1111 Help

Select chemical process

- Aluminum etch type A (Transene)
- Chromium etchant (Transene 1020)**
- MF-312 developer + DI water
- Microchem MBK:IPA 1:3
- PGMEA
- Acetone, Methanol, IPA

Description/precautions

Nitric acid/ceric ammonium nitrate aqueous solution
 Main hazards: Oxidizing, corrosive, toxic, skin burns
 Main controls: Perform work inside hood, wear nitrile gloves over cleanroom gloves, goggles

Comments

Waste bottle code: **A-I-2**

MAP OF WASTE LOCATIONS SOP MSDS

START PROCESS Approx. amount (ml) 0 END PROCESS

CANCEL/RESET

For staff use only ADD/EDIT USER ADD/EDIT WASTE REVIEW

Figure 2. Software user interface. A-I-2 is the chemical waste bottle code for the selected process. The three commands at the bottom of the interface are used by staff to perform diverse administrative actions, such as adding users and chemical processes to the software's database.

Figure 3. Map of locations of waste cabinets.

Before pressing the START PROCESS button (see Fig. 2), users must verify the physical location of the chemical waste container. Also, they must check that it can accommodate the amount of waste they plan to generate. If these conditions are not met, users have to contact a lab staff member; otherwise, users acknowledge the beginning of the chemical process by pressing the START PROCESS button in the user interface. This action sets the user status in the system as “ongoing,” which is used for monitoring purposes as will be described in the next section, and automatically logs off the user from the software. Users can set multiple ongoing chemical processes, which is useful when performing back-to-back processes that generate incompatible waste, like, for example, photoresist developing followed by chemical etching.

After completion of a chemical process and disposal of the generated waste, users log on to finalize their sessions. Users are presented with the pop-up window shown in Fig. 4, in which they can either start a new process or finish “ongoing” ones. Selecting an ongoing process and pressing the END ONGOING PROCESS button brings back the user interface, in which users input the estimated waste volume (see Fig. 5). Clicking the END PROCESS button finishes (removes the ongoing status) the selected process and automatically logs off the user from the software.

Figure 4. Pop-up window in which users can start a new chemical process or end an ongoing one.

Figure 5. User interface presented to users after clicking the END ONGOING PROCESS button in Fig. 4. The END PROCESS button signals the termination of an ongoing chemical process.

3. Results and discussion

The software has been implemented since 2010 in the cleanroom of the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory in New York, which hosts over 150 users per year. It has been an important factor for preventing chemical accidents that are caused by misplacement of chemical waste in incompatible containers. Since its implementation, the CFN has had only one recorded incident of the above nature,² which occurred when a user by-passed the software's work flow described in Fig. 1.

This excellent safety record is due to the training offered to CFN users and to the continued supervision by the cleanroom staff. A tool that has been very helpful at enforcing the software's workflow is the installation of monitors, inside and outside the cleanroom, displaying a list of the ongoing chemical processes (Fig. 6). This information helps users to plan their work and also lets them anticipate potential hazardous situations. In addition, these monitors allow staff to verify if users are complying with the prescribed workflow in Fig. 1.

User name	date in	Process
Nathalie Linda	7/14/2016	MF-312 developer
Jose Huang	7/14/2016	Microchem MIBK:IPA 1:3
Fernando Camino	7/14/2016	Chromium etchant (Transene 1020)

Figure 6. Screenshot of the list of ongoing chemical processes, which is displayed in a couple of stand-alone monitors inside and outside the cleanroom.

4. Summary

We have implemented a software for logging chemical processes in the cleanroom of the Center for Functional Nanomaterials at Brookhaven National Laboratory in New York. The software allows users to perform only those processes displayed in their list of authorized chemical processes. Once a user selects a chemical process, the software gives the location and label code of the corresponding chemical waste container. This software has been effective at avoiding hazardous situations connected with the disposal of chemical waste in incompatible waste containers, which consists of an important cause of accidents in chemical laboratories.

Acknowledgements

This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704. The authors are thankful to Dr. Charles Black and Dr. James Dickerson for their support in implementing the software in the Center for Functional Nanomaterials. Special thanks to the nanofabrication facility staff—Gwen Wright, Aaron Stein and Ming Lu—for adopting and improving the software, and to Wai-Lin Ng and Edward Sierra for their comments on the manuscript.

References

- [1] For a comprehensive review of authorized work and other chemical safety concepts and recommendations, see e.g., National Research Council. *Prudent Practices in the Laboratory*:

Handling and Management of Chemical Hazards, Updated Version. The National Academies Press: Washington, DC, 2011. doi:10.17226/12654.

- [2] Incident reported in the Department of Energy Occurrence Reporting and Processing System (ORPS), with ID: SC-BHSO-BNL-BNL-2014-0016.