

**EMISSION FACTOR OF VOCs FROM NON-POINT SOURCE:
CASE STUDY OF CHEMICAL LABORATORY**

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Thesis
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EMISSION FACTOR OF VOCs FROM NON-POINT SOURCE:
CASE STUDY OF CHEMICAL LABORATORY

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ABSTRACT

The emission factors, used to estimate the release of chemicals into the environment were researched in this study. These emission factors were obtained from direct measurements and were calculated as emission rates, expressed in the unit of kg of release per 1000 kg of chemical used.

In this study, the emission factors of three scientific analytical laboratories were studied. The release of chemicals from a school, a university and a commercial laboratory were estimated. The results from the study in the school using ethyl acetate found that emission factors to air were 383.09 and 174.13 kg/1000 kg for open and closed laboratory conditions, respectively. As for the university, analytical results using ethyl acetate found that the emission rate to air was 445.53 kg/1000 kg. Emission factors to air of the commercial laboratory using isopropyl alcohol and toluene were 2.20 and 10.77 kg/1000 kg, respectively. The study results indicated the emission rate from the open-room condition was higher than the closed-room condition. The lowest emission rate was estimated at the commercial laboratory. Good practice and using of appropriate VOC control equipment were found to reduce the emission of VOCs from this laboratory.

Releases of chemicals to other environmental media were estimated by using mass balance calculation. The emission rate of ethyl acetate to water from the school's laboratory was estimated as 119.40 and 328.36 kg/1000 kg for open-room and closed-room conditions, respectively. There were no releases of chemicals to waste. The emission rate of ethyl acetate to waste from the university's laboratory was 425.75 kg/1000 kg. There was no emission to water. As for the commercial laboratory, the emission rates of isopropyl alcohol and toluene to waste were estimated as 497.80 and 489.23 kg/1000 kg, respectively. There were no emissions to water from this source.

KEY WORDS: CHEMICAL LABORATORY /EMISSION FACTOR /VOCs /
NON-POINT SOURCE /PRTR

116 pages

Emission factor ของสารประกอบอินทรีย์ระเหยจากแหล่งกำเนิดที่ไม่ใช่ปล่อง กรณีศึกษาในห้องปฏิบัติการเคมี
EMISSION FACTOR OF VOCs FROM NON-POINT SOURCE: CASE STUDY OF CHEMICAL
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บทคัดย่อ

งานวิจัยนี้เป็นการพัฒนาค่า emission factor เพื่อใช้ในการประเมินปริมาณการระบายสารเคมีออกสู่สิ่งแวดล้อม โดยค่า Emission factor นี้ได้มาจากการตรวจวัดโดยตรง และคำนวณออกมาเป็นอัตราการระบายสารเคมีสู่สิ่งแวดล้อมในหน่วยกิโลกรัมของสารต่อ 1000 กิโลกรัมที่ใช้

การศึกษานี้เป็นการพัฒนาค่า Emission factor จากแหล่งกำเนิดจำพวกห้องปฏิบัติการทางวิทยาศาสตร์ โดยทำการศึกษาและคาดการณ์ปริมาณการปลดปล่อยสารเคมีของห้องปฏิบัติการ โรงเรียนมหาวิทยาลัย และห้องปฏิบัติการเอกชน ผลการศึกษาในห้องปฏิบัติการของโรงเรียน โดยการทดสอบกับสารเอทิลอะซีเตทพบว่าค่า Emission factor ที่ระบายออกสู่อากาศ เท่ากับ 383.09 และ 174.13 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม สำหรับกรณีห้องปฏิบัติการในระบบเปิดและระบบปิดตามลำดับ ในส่วนของห้องปฏิบัติการมหาวิทยาลัย ผลการศึกษาโดยการทดสอบกับสารเอทิลอะซีเตท พบว่า มีอัตราการระบายสู่อากาศ เท่ากับ 445.53 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม และผลการศึกษาในห้องปฏิบัติการเอกชนโดยใช้สารไอโซโพรพิลแอลกอฮอล์ และโทลูอิน พบว่าอัตราการระบายสู่อากาศ เท่ากับ 2.20 และ 10.77 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม ตามลำดับ ผลจากการศึกษาพบว่าห้องปฏิบัติการระบบเปิดมีอัตราการปลดปล่อยสารออกสู่อากาศมากกว่าระบบปิด และอัตราการระบายน้อยที่สุดพบในห้องปฏิบัติการเอกชน เนื่องจากการปฏิบัติการที่ดีและการติดตั้งระบบบำบัดจะช่วยลดปริมาณการปลดปล่อยสารเคมีออกสู่อากาศ

การคาดการณ์ปริมาณการปลดปล่อยสารออกสู่สิ่งแวดล้อมอื่นๆ ได้จากการคำนวณสมมูลมวล ในส่วนห้องปฏิบัติการของโรงเรียนพบว่าปริมาณการปลดปล่อยสารเอทิลอะซีเตทออกสู่น้ำเท่ากับ 119.40 และ 328.36 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม (กรณีห้องเปิด และห้องปิด) และไม่มีการเคลื่อนย้ายไปสู่ของเสีย ในส่วนห้องปฏิบัติการของมหาวิทยาลัยพบว่าปริมาณการปลดปล่อยสารเอทิลอะซีเตทออกสู่ของเสียเท่ากับ 425.75 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม และไม่มีการปลดปล่อยออกสู่น้ำ ส่วนของห้องปฏิบัติการเอกชนพบว่าปริมาณการปลดปล่อยสารไอโซโพรพิลแอลกอฮอล์ และโทลูอินออกสู่ของเสียเท่ากับ 497.80 และ 489.23 กิโลกรัมต่อปริมาณการใช้สาร 1000 กิโลกรัม และไม่มีการปลดปล่อยออกสู่น้ำจากแหล่งกำเนิดดังกล่าว

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CHAPTER I

INTRODUCTION

1.1 Rationales and justifications

In Thailand, rapid industrialization and urbanization have brought about not only prosperity to the country, but also severe pollution problems. To tackle the issue, the Pollution Control Department (PCD), Ministry of Natural Resources and Environment, has established environmental quality standards for basic air pollutants such as sulfur oxides and suspended particulate matters, and has been conducting monitoring in Bangkok and in the whole country.

As for measures to address volatile organic compounds (VOCs), Thailand has established environmental and emission standards for a number of selected VOCs. A systematic monitoring of targeted VOCs and proposed environmental and emission standards of VOCs were proposed. The next step for Thailand is to provide comprehensive management of chemical risks and environmental information.

Pollutant Release and Transfer Register (PRTR) is the database of type and amount pollutants release to environment and pollutants transfer between media. In the recent year, Japan, USA, and some country in Europe use PRTR system application to reduce confliction among population and trader. The government uses this system for environment management and controlling of pollution sources. (OECD, 1996)

PRTR is such management system as operated in all the member countries of Organization for Economic Co-operation and Development (OECD). Under PRTR system, emission of selected chemical substances are reported by point sources (usually industry) and estimated for non-point sources (such as mobile and household) by the government. Then the data are to be compiled and presented to public for better understanding of chemical substances in environment. Thus, PRTR can promote constructive dialogue among all the stakeholders.

Emission sources can be divided into two types namely point source; industrial plant, tank farm and non-point source; vehicle, agriculture. In PRTR system point source makes a report and submits it to the government. As for non-point source, the government is responsible for estimation of these data.

Laboratories use chemical substance for an experimental analysis which may release chemical into environment media; air, water and soil. The management of chemical is interested to prevent and protect people who work in this area. The management of chemical reagents has become an important issue in preserving the environment and the health of students and researchers. (Nomura et al, 2006)

This study estimated the emission factor of target chemical from laboratory institutions on the basis of direct measurement and chemical mass balance. The losses of chemicals in laboratories due to volatility were evaluated and the emission rates of chemicals to environmental media were developed.

1.2 Research objectives

To develop emission factor and estimate the release and transfer quantity of the target PRTR chemicals from laboratory activities.

1.3 Scope of study

Target chemical was selected from 107 substances of Thai's PRTR. Selection of target chemical was based on amount of used and toxic to health.

Pilot laboratory: three pilot laboratories were selected in this study. They were as follows:

- 1) High school: Rayong Wittayakom school
- 2) University: Central laboratory, Faculty of Public Health, Mahidol University
- 3) Commercial laboratory: PTT-Global Chemical Co.,Ltd.

Target chemicals:

- 1) Ethyl acetate: Rayong Wittayakom school, Mahidol University
- 2) Isopropyl alcohol: PTT-Global Chemical Co.,Ltd.
- 3) Toluene: PTT-Global Chemical Co.,Ltd.

1.4 Expected outcomes

Emission factor of chemical released from laboratory activities and identification of good practices for laboratory in order to minimize emission of chemicals to the environment

1.5 Conceptual framework

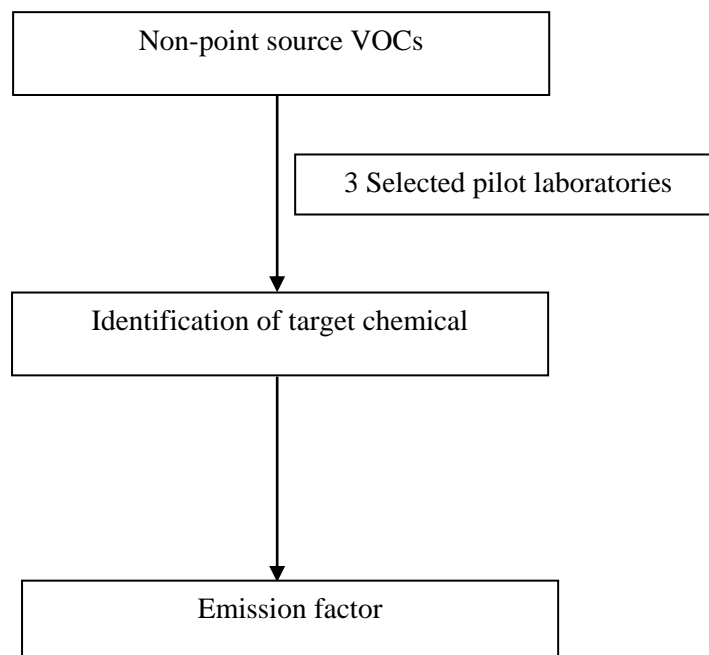


Figure 1.1 Conceptual framework

CHAPTER II

LITURATURE REVIEWS

2.1 Pollutant Release and Transfer Register (PRTR)

2.1.1 Definition of PRTR

A Pollutant Release and Transfer Register (PRTR) is a catalogue or register of potentially harmful pollutant releases or transfers to the environment from a variety of sources. A PRTR includes information about releases or transfers to air, water and soil as well as about wastes transported to treatment and disposal sites. This register also consists of reports about specific species such as benzene, methane or mercury as contrasted with broad categories of pollution such as volatile organic compounds, greenhouse gases or heavy metals. The development and implementation of a PRTR system is adapted to national needs represents a means for governments to track generation, release and the fate of various pollutants over time. (OECD, 1996)

A PRTR can be an important tool in the total environment policy of a government – providing otherwise difficult to obtain information about the pollution burden, encouraging reporters to reduce pollution, and engendering broad public support for government environmental policies. Indeed, governments may wish to set forth long-term national environmental goals to promote sustainable development and then use PRTR as an important tool to examine objectively how well these goals are being met. (OECD, 1996)

2.1.2 Benefits of a PRTR

One of the reasons for the success of PRTR systems is that they entail benefits and possible uses for government, reporting industries and members of the public: (OECD, 1996)

➤ Benefits to Government

- Identification of who is generating potentially harmful chemical releases, what type of pollutants are being released, quantities of those releases, and to what media these pollutants are being released;
- Identification of geographic areas of concern;
- Facilitation of decisions on environmental management priorities;
- Facilitation of the measurement of national progress toward risk reduction and pollution prevention goals; and
- Monitoring enforcement of current regulation and fulfilling international reporting requirements under various international convention and agreements.

➤ Benefits to Industry

- Identification of sources of lost revenue in their industrial processes;
- Implementation of improved chemical use controls and increased equipment efficiency;
- Incentive implementation of cleaner production schemes;
- Increase of competitiveness;
- Incentive transfer of technology within and among companies; and
- Serve as a catalyst for better communication and relations between plants and neighboring communities, establishing trust and confidence.

➤ Benefits to the Public

- Entitlement to know about potential risks from chemicals in their communities;
- Enhancement of the right to make informed choices and take appropriate actions regarding pollution;
- Incentive own measures of workers to protect themselves and their facilities from chemical-related accidents; and
- Increase public participation on environmental decision-making.

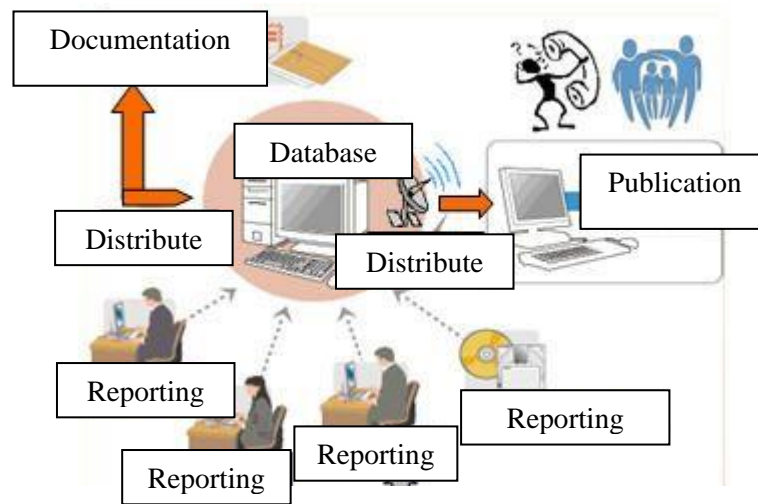


Figure 2.1 PRTR system
(OECD, 1996)

2.2 Laboratory

A laboratory is a facility that provides controlled conditions in which scientific research, experiments, and measurement may be performed. Lab is used for scientific research take many forms because of the differing requirements of specialists in the various fields of science. A physics lab might contain a particle accelerator or vacuum chamber, while a metallurgy lab could have apparatus forecasting or refining metals or for testing their strength. A chemist or biologist might use a wet laboratory, while a psychologist's lab might be a room with one-way mirrors and hidden cameras in which to observe behavior. In some laboratories, such as those commonly used by computer scientists, computers (sometimes supercomputers) are used for either simulations or the analysis of data collected elsewhere.

Despite the great differences among laboratories, some features are common. The use of workbenches or countertops at which the scientist may choose to either sit or stand is a common way to ensure comfortable working conditions for the cabinets for the storage of laboratory equipment is quite common. It is traditional for a scientist to record an experiment's progress in a laboratory notebook, but modern labs almost always contain at least one computer workstation for data collection and analysis.

Scientific laboratories can be found in schools and universities, in industry, in government or military facilities, and even aboard ships and spacecraft. A laboratory might offer work space for just one to more than thirty researchers depending on its size and purpose. Recently, a new type of laboratory called Open Laboratory has emerged. Its format allows the sharing of space, equipment, support staff between different research groups and also fosters information exchange through communications across fields. (Michael et al., 2007)

2.3 Chemical substances

A chemical substance is a form of matter that has constant chemical composition and characteristic properties. (IUPAC, 1997) Chemical substances (also called pure substances) may well be defined as "any material with a definite chemical composition" (Hill et al., 2005) According to this definition a chemical substance can either be a pure chemical element or a pure chemical compound. However, there are exceptions to this definition; a pure substance can also be defined as a form of matter that has both definite composition and distinct properties. The chemical substance index published by CAS also includes several alloys of uncertain composition. (Diracdelta, 2013) Non-stoichiometric compounds are a special case (in inorganic chemistry) that violates the law of constant composition, and for them, it is sometimes difficult to draw the line between a mixture and a compound, as in the case of palladium hydride. Broader definitions of chemicals or chemical substances can be found, for example: "the term 'chemical substance' means any organic or inorganic substance of a particular molecular identity, including – (i) any combination of such substances occurring in whole or in part as a result of a chemical reaction or occurring in nature"(USEPA, 2009)

2.4 PRTR target chemical

In Thailand, there are 107 chemical substances required estimation of their release and transfer amount under the PRTR program. The list of these target chemicals is as shown in Table 2.1.

Table 2.1 List of PRTR target chemical.

No.	Name of Chemical	CAS No.	Note : Reason for selection
1	1-(p-Methoxyphenyl)-2-methyl-1,3-propanediol-methylene ether	5689-72-5	HS Act class 3 and over 1000 ton/year.
2	2,4-D-dimethylammonium	2008-39-1	HS Act class 3 and over 1000 ton/year.
3	2, 4-D-butotyl	1929-73-3	HS Act class 3 and over 1000 ton/year.
4	2, 4-D-butyl	94-80-4	HS Act class 3 and over 1000 ton/year.
5	Acetaldehyde	75-07-0	Carcinogen data on US EPA and frequent detection in monitoring.
6	Acetone	67-64-1	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
7	Acrylamide	79-06-1	HS Act class 2, Carcinogen data on US EPA and over 100 ton/year.
8	Acrylic acid	79-10-7	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
9	Acrylonitrile	107-13-1	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
10	Ametryn	834-12-8	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
11	Antimony and its compounds		Quantitative toxic data on US EPA and over 1000 ton/year.
12	Arsenic and its compounds		HS Act class 3, Carcinogen data on US EPA as Arsenic and approx. 80 ton/year. Expert judgment.
13	Atrazine	1912-24-9	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
14	Benzene	71-43-2	HS Act class 3, Carcinogen data on US EPA and frequent detection in monitoring.
15	Benzyl chloride	100-44-7	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
16	Bis(2-ethylhexyl)phthalate	117-81-7	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
17	Bisphenol A	80-05-7	Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
18	Boron and its compounds		HS Act class 3 and over 1000 ton/year.
19	Bromo-2-chloroethane, 1-	107-04-0	Carcinogen data on US EPA and over 100 ton/year.
20	Butachlor	23184-66-9	HS Act class 3 and over 1000 ton/year.
21	Butadiene, 1,3-	106-99-0	HS Act class 3, Carcinogen data on US EPA and frequent detection in monitoring.
22	Cadmium and its compounds	7440-43-9	HS Act class 3, 4 and over 1000 ton/year.
23	Captan	133-06-2	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
24	Carbon disulfide	75-15-0	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
25	Chloroacetaldehyde, 2-	107-20-0	Carcinogen data on US EPA and over 100 ton/year.
26	Chloroacetic acid	79-11-8	Quantitative toxic data on US EPA and over 1000 ton/year.
27	Chloroform (trichloromethane)	67-66-3	HS Act class 3-4, Carcinogen data on US EPA and approx. 80 ton/year. Expert judgment.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
28	Chlorothalonil	1897-45-6	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
29	Chlorpyrifos	2921-88-2	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
30	Copper and soluble salts		HS Act class 3 and over 1000 ton/year.
31	Cromium and its compounds		HS Act class 3, Carcinogen data on US EPA as Cr(VI) and over 100 ton/year.
32	Cyclohexanone	108-94-1	Quantitative toxic data on US EPA and over 1000 ton/year.
33	Dialifos (Dialifor)	10311-84-9	HS Act class 3 and over 1000 ton/year.
34	Dichlorobenzene, 1,4	106-46-7	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
35	Dichloroethane, 1,2-	107-06-2	HS Act class 3-4, Carcinogen data on US EPA and over 100 ton/year.
36	Dichlorophenoxy acetic acid, 2,4-	94-75-7	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
37	Dichlorvos	62-73-7	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
38	Diethylene glycol monobutyl ether	112-34-5	Quantitative toxic data on US EPA and over 1000 ton/year.
39	Dithiopyr	97886-45-8	HS Act class 3 and over 1000 ton/year.
40	Epichlorohydrin	106-89-8	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
41	Ethyl acetate	141-78-6	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
42	Ethyl acrylate	140-88-5	HS Act class 2, Carcinogen data on US EPA and over 100 ton/year.
43	Ethylene glycol	107-21-1	Quantitative toxic data on US EPA and over 1000 ton/year.
44	Ethylene glycol monobutyl ether	111-76-2	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
45	Ethylene oxide	75-21-8	HS Act class 4, Carcinogen data on US EPA and over 100 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
46	Formaldehyde	50-00-0	HS Act class 2, Carcinogen data on US EPA and over 100 ton/year.
47	Formic acid	64-18-6	Quantitative toxic data on US EPA and over 1000 ton/year.
48	Furfural	98-01-1	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
49	Glyphosate-isopropylammonium	38641-94-0	HS Act class 3, and over 1000 ton/year.
50	Hexachlorocyclohexane	319-86-8	Carcinogen data on US EPA and over 100 ton/year.
51	Hexane, N-	110-54-3	Quantitative toxic data on US EPA and over 1000 ton/year.
52	Hexanedioic acid	124-04-9	Quantitative toxic data on US EPA and over 1000 ton/year.
53	Hydrogen fluoride	7664-39-3	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
54	Hydroquinone	123-31-9	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
55	Imazaquin-ammonium	81335-47-9	HS Act class 3 and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
56	Isobutyl alcohol	78-83-1	Quantitative toxic data on US EPA and over 1000 ton/year.
57	Isophorone	78-59-1	Carcinogen data on US EPA and over 100 ton/year.
58	Isopropyl alcohol	67-63-0	Quantitative toxic data on US EPA and over 1000 ton/year.
59	Lead and compounds	7439-92-1	Quantitative toxic data on US EPA and over 1000 ton/year.
60	Maleic anhydride	108-31-6	Quantitative toxic data on US EPA and over 1000 ton/year.
61	Manganese and its compounds		HS Act class 1 and over 1000 ton/year.
62	Methanol	67-56-1	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
63	Methyl acetate	79-20-9	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
64	Methyl acrylate	96-33-3	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
65	Methyl ethyl ketone (2-butanone)	78-93-3	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
66	Methyl isobutyl ketone (4-methyl-2-pentanone)	108-10-1	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
67	Methyl methacrylate	80-62-6	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
68	Methyl tert-butyl ether (MTBE)	1634-04-4	Carcinogen data on US EPA and over 100 ton/year.
69	Methylene chloride	75-09-2	HS Act class 1, Carcinogen data on US EPA and over 100 ton/year.
70	Methylenediphenyl diisocyanate	101-68-8	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
71	Molybdenum and its compounds		Quantitative toxic data on US EPA and over 1000 ton/year.
72	Naphthalene	91-20-3	HS Act class 2, Carcinogen data on US EPA and over 100 ton/year.
73	Nickel and its compounds		Carcinogen data as NiCl ₂ on US EPA and over 100 ton/year.
74	Paraquat dichloride	1910-42-5	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
75	Pentane, n-	109-66-0	Quantitative toxic data on US EPA and over 1000 ton/year.
76	Phenol	108-95-2	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
77	Phosphoric acid	7664-38-2	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
78	Phosphorus pentoxide and other	1314-56-3	HS Act class 3 and over 1000 ton/year.
79	Phthalic anhydride	85-44-9	Quantitative toxic data on US EPA and over 1000 ton/year.
80	Polyethylene glycol nonylphenyl ether	9016-45-9	HS Act class 3 and over 1000 ton/year.
81	Potassium chlorate	3811-04-9	HS Act class 3 and over 1000 ton/year.
82	Propanil	709-98-	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
83	Propionic acid	79-09-4	HS Act class 3 and over 1000 ton/year.
84	Propylene	115-07-1	Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
85	Propylene glycol	57-55-6	Quantitative toxic data on US EPA and over 1000 ton/year.
86	Propylene oxide	75-56-9	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
87	Prothiocarb	19622-08-3	HS Act class 3 and over 1000 ton/year.
88	Pyrene	129-00-0	HS Act class 1, Quantitative toxic data on US EPA and over 1000 ton/year.
89	Ryania	15662-33-6	HS Act class 3 and over 1000 ton/year.
90	Sodium chlorate	7775-09-9	HS Act class 3-4 and over 1000 ton/year.
91	Sodium cyanide	143-33-9	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.
92	Styrene	100-42-5	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
93	Tebuthiuron	34014-18-1	HS Act class 3, Quantitative toxic data on US EPA and over 1000 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
94	Tetrachloroethylene	127-18-4	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.
95	Tin and its compounds		Quantitative toxic data on US EPA and over 1000 ton/year.
96	Toluene	108-88-3	HS Act class 3, Quantitative toxic data on US EPA and frequent detection in monitoring.
97	Trichloroethylene	79-01-6	HS Act class 1, Carcinogen data on US EPA and over 100 ton/year.
98	Trimethylbenzene, 1,2,4-	95-63-6	Quantitative toxic data on US EPA and over 1000 ton/year.
99	Trimethylbenzene, 1,3,5-	108-67-8	Quantitative toxic data on US EPA and over 1000 ton/year.
100	Trinitrotoluene, 2,4,6-	118-96-7	Carcinogen data on US EPA and over 100 ton/year.
101	Vinyl acetate	108-05-4	HS Act class 2, Quantitative toxic data on US EPA and over 1000 ton/year.
102	Vinyl chloride	75-01-4	HS Act class 3, Carcinogen data on US EPA and over 100 ton/year.

Table 2.1 List of PRTR target chemical.(cont.)

No.	Name of Chemical	CAS No.	Note : Reason for selection
103	Xylenes		Quantitative toxic data on US EPA and over 1000 ton/year.
104	Zinc and its compounds		Quantitative toxic data on US EPA and over 1000 ton/year.
105	SO _x		To be included in data disclosure to public. Not required for industry reporting as regulation already exist for reporting.
106	NO _x		To be included in data disclosure to public. Not required for industry reporting as regulation already exist for reporting.
107	Dioxin and Furan		To be included in the system when the reliable data become available for their emission status and factors. Not included for the pilot project.

Note: HS Act = Hazardous Substance Act

2.5 Emission Factor

Emissions factors have long been the fundamental tool in developing national, regional, state, and local emissions inventories for air quality management decisions and in developing emissions control strategies. Recently, emissions factors have been applied in determining site-specific applicability and emissions limitations

in operating permits by both private and government authorities. (USEPA, 1995) These users have requested guidance on the use of emissions factors and other emissions quantification tools (e.g., emissions testing and monitoring, mass balance techniques) in developing permits that are practical in their enforcement.

An emissions factor is a representative value that attempts to relate the quantity of a pollutant released to the atmosphere with an activity associated with the release of that pollutant. These factors are usually expressed as the weight of pollutant divided by a unit weight, volume, distance, or duration of the activity emitting the pollutant (e.g., kilograms of particulate emitted per megagram of coal burned). Such factors facilitate estimation of emissions from various sources of air pollution. In most cases, these factors are simply averages of all available data of acceptable quality, and are generally assumed to be representative of long-term averages for all facilities in the source category (i.e., a population average).

The general equation for emissions estimation is:

Where:

$E = A \times EF \times (1 - ER/100)$	equation (2.1)
---------------------------------------	----------------

E = emissions;

A = activity rate;

EF = emission factor, and

ER = overall emission reduction efficiency, %

AP-42, *Compilation of Air Pollutant Emission Factors*, has been published since 1972 as the primary compilation of USEPA's emission factor information. It contains emission factors and process information for more than 200 air pollution source categories. A source category is a specific industry sector or group of similar emitting sources. The emission factors have been developed and compiled from source test data, material balance studies, and engineering estimates. (USEPA, 1995)

2.6 Related research

Nomura *et al.*, (2006) studied release and transfer of chemical substances in Japanese University. These chemicals were thought to be volatilized mainly through

reduced pressured distillation. However, it was found that loss of chemicals was mainly due to volatility, which researchers were unaware of, such as that during solvent recovery under reduced pressure and volatilization from containers of organic waste liquid.

Cynthia *et al.*, (2011) studied the reliability and accuracy of test use to measure emission of volatile organic compounds (VOCs) from samples of interior building products. The National Institute of Standards and Technology (NIST) and Virginia Tech (VT) created a program to develop reference materials with independently predictable emission rates. The success of this pilot ILS was a key step toward being able to provide a VOC reference material for independent validation of VOC emission tests conducted in small chambers.

Mingang *et al.*, (2012) studied chemical spills occur frequently in laboratories. The current ventilation code for laboratories recommends a ventilation rate of 12 ACH for maintaining a safe laboratory environment. This experimental study investigated the ventilation performance under different ventilation rates in a chemistry laboratory mockup. The impact of wall exhaust locations and chemical spill positions was examined related to the contaminant concentration distribution in the laboratory. This investigation also studied the ventilation performance with and without the use of bench hood exhausts. The results showed that the contaminant concentration was not linearly proportional to the ventilation rate. If the chemical spill position was close to an exhaust, the contaminant concentration in the laboratory could be rather low. The bench hood exhaust had the potential to effectively reduce the contaminant concentration. The results indicated that the ventilation rate in a chemistry laboratory may be reduced without increasing the safety risk if the ventilation system is properly designed.

Ke *et al.*, (2012) studied pollutant dilution by mean of variation of ventilation. Results showed that for reducing the concentration in the lower zone to a certain value, the concentration of inflow air and indoor emission rate should be less than their critical values for a given effective opening area of the window. The effect of thermal radiation of the inner surface on the reduction of pollutant concentration in the upper zone is greater than that in the lower zone of displacement natural ventilation (DNV) room. In addition, the effective opening area of the window

primarily influences the final concentration level in the DNV room, and only affects the decay rate of indoor pollutant concentration when the pollutant concentration of incoming air or the strength of the indoor source approach their critical values.

Tan *et al.*, (1999) conducted their comparative study in two laboratory types in Massachusetts Institute of Technology (MIT), teaching lab for undergraduate students and research laboratories for graduate students and research staff. The objective of this study was to determine chemical exposures during teaching and research activities. Air samples were collected from both teaching and research laboratories in the departments of Material Sciences and Engineering, Chemical Engineering, and Biology. The most frequently sampled chemicals in these three departments were cobalt, styrene, and formaldehyde, respectively. A total of 23 different agents were measured. There were 70 samples from teaching laboratories, and 62 samples from research laboratories. The chemical exposures relative to the standards in teaching laboratories were statistically higher than in research laboratories. Information about personal protective equipment and the use of laboratory chemical hoods was also collected. The differences in use of personal protective equipment (PPE) among these departments were not statistically significant. Results of this study were found that (1) Chemical exposures in the academic laboratories in this study were all well below the health standards; (2) Undergraduate students in teaching laboratories had higher chemical exposures than graduate students in research laboratories; (3) Chemical exposures among departments were not significantly different; and (4) Hazard communication, safety training, and laboratory rules enforcement are important for protection and may be the reason that the results from this study indicated that chemical exposures in this academic institution were well below the health standards under normal operations.

Zhang *et al.*, (2003) found that the building envelopes are usually comprised of layer with different materials, which can significantly affect volatile organic compounds (VOCs) concentrations in indoor environments. These layers may act as source and sink alternatively depending on the different sorption and diffusion potentials. The model proposed here is a single zone one and it considers the different emission properties of building components, namely, the different sorption and diffusion characteristics of the side walls, the floor and the ceiling. In addition, each

component comprises of several layers, which represents different construction materials. Two VOCs, ethyl acetate and n-octane, representing polar and nonpolar compounds respectively, are modeled to study the emission profiles in a room with several building materials. The effects of various construction materials, and the different convective mass transfer coefficients between room air and different building components, on the emission characteristics are investigated.

Uhde *et al.*, (1998) studied the Field and Laboratory Emission Cell (FLEC) in order to design material for VOC emission testing. Knowledge about the air flow field in the cell compartment is highly desired, as the air velocity at the sample surface may considerably influence the emission behavior. A simple mathematical approach of flow theory predicted an unevenly distributed air flow into the FLEC. This could be confirmed by air velocity measurements using a self-constructed hot-wire anemometer. With a total flow of 250 mL/min, air velocities measured at the surface ranged from ≤ 0.1 to 0.9 cm/s. A surface area of very low air velocities was detected in the FLEC center with a radius of ≈ 20 mm. A VOC emission test using a simulated punctual source yielded different emission rates at different locations in the cell compartment.

Takada *et al.* (2007) studied research laboratories in a university were investigated for air-borne levels of legally designated organic solvents and specified chemical substances. Repeated surveys in 2004-2005 (four times in the two years) of about 720 laboratories (thus 2,874 laboratories in total) revealed that the solvent concentrations were in excess of the Administrative Control Levels only in a few laboratories (the conditions improved shortly after the identification) and none with regard to specified chemicals. Thus, working environments were in Control Class 1 in almost all (99.5%) laboratories examined. Such conditions were achieved primarily by extensive installation and use of local exhaust systems. The survey further revealed that types of chemicals used in research laboratories were extremely various (only poorly covered by the regulation) whereas the amounts of each chemical to be consumed were quite limited. For protection of health of researchers (including post- and under-graduate students) in laboratories, therefore, it appeared more appropriate to make personal exposure assessment rather than evaluation of levels of chemicals in air of research laboratories. Considering unique characteristics of research activity, it is

important to educate each researcher to make his/her own efforts to protect his/her health, through supply of knowledge on toxicity of chemicals as well as that on proper use of protective equipment including exhaust chambers.

Christophe *et al.*, (2010) studied six European laboratories used the emission test chamber method (EN ISO 16000-9) for the determination of VOC and formaldehyde emissions from a wood based panel (particleboard). The tested panel was conditioned without wrapping over 28 days at 23°C and 50% RH before shipping to each participating laboratory. Emission chamber testing was carried out with air sampling after 3 and 28 days. Main VOCs (alpha-pinene, beta-pinene, pentanal, hexanal) and TVOC were analysed according to ISO 16000-6 and main aldehydes (formaldehyde, acetaldehyde, pentanal, hexanal) were specifically analysed according to ISO 16000-3. Results indicated that relative standard deviations of reproducibility after 28 testing days are between 27.5% and 45.5% for VOC concentrations ranging from 5.9 to 38.6 $\mu\text{g}/\text{m}^3$ and between 17.1% and 23.8% for aldehyde concentrations ranging from 5.5 to 57.6 $\mu\text{g}/\text{m}^3$. Formaldehyde results showed standard deviation of only 17.4% for a mean concentration of 57.6 $\mu\text{g}/\text{m}^3$ after 28 testing days. In general, results are similar to recent inter-laboratory comparison studies even if wood based panels can be considered as heterogeneous materials.

CHAPTER III

METHODOLOGY

3.1 Selection of pilot laboratories

Pilot laboratory in this study consists of the chemical laboratory of high school, university and private (commercial) laboratory.

High school, selected as pilot laboratory in this study is Rayong Wittayakom school, located in Rayong province. This school has the highest number of high school student (grade 10-12) in Rayong province.

As for university laboratory, the central laboratory of the Faculty of Public Health, Mahidol University in Bangkok is selected as pilot laboratory. The private (commercial) laboratory in this study is analytical laboratory of PTT Global Chemical Co.,Ltd. (PTT-GC), located in Rayong province.

3.2 Target chemicals

The target chemicals in this study are set in accordance with target chemical, listed in the Pollutant Release and Transfer Registration (PRTR). In total, there are 107 chemical compounds under the PRTR program. The lists of these chemicals are as shown in Table 2.1.

List of PRTR chemicals are used together with the list of substances, used in each laboratory. The carcinogenic characteristics and amount of usage of chemical substance are used as parameters in the selection matrix as shown in Table 3.1. In the selection matrix, a compound, considered as carcinogen or having high amount of usage (>10% of PRTR reporting criteria of 1000 kg/year = 100 kg/year) will be selected. Estimations of release and transfer of these chemical to environmental media are carried out by direct measurement and mass balance analysis.

Table 3.1: Example of selection matrix of target chemical

Target Chemical of PRTR (107 substances)	Chemical in laboratory	Carcinogenic criteria (IARC)	Amount of usage (kg/year)	Selection
Ethyl acetate	✓	-	104	✓
Formaldehyde	✓	Group 1	83	
Hexane	✓	-	256	✓
Methanol	-	-	-	
Naphthalene	✓	Group 2B	39	

- Selection criteria

Toxicity: by Carcinogen classification (IARC) group 1 and 2A

Amount of usage: >10% PRTR’s requirement for reporting (1000 kg/year)
= 100 kg/year

3.3 Target chemical emission assessment

3.3.1 Mass flow estimation for PRTR

The mass balance of selected target chemical in pilot laboratory was determined as summarized in Figure 3.1. Details are as follows:

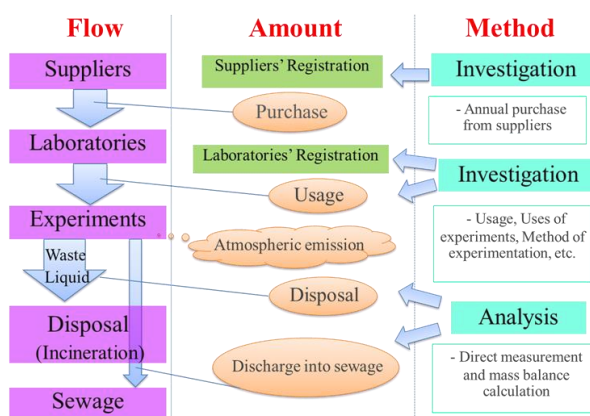


Figure 3.1 The chemical flow and survey method. (adapted from Nomura et al., 2006)

- Investigation at suppliers

Annual purchase of selected target chemical is obtained from chemical supplier of each laboratory.

- Investigation at laboratories

Collected data are consumption amount of target chemical substances in the experiment, data regarding the purchase, usage of chemicals and handing of chemicals by using survey sheets.

- Disposal amount

Laboratory wastes are sent to authorize companies for disposal. Survey sheet is distributed to companies.

- Discharge to sewage

The amount of discharge is estimated on the basis of chemical concentrations and drainage volume.

- Atmospheric emissions

Target chemical can be volatile to air. These emissions are calculated by subtracting the amounts disposed of and discharged from the amount used. Atmospheric emission of selected target chemicals is determined by measuring the air concentration of chemical in hood or experimental area during laboratory process.

3.3.2 Estimation of possessed amount of target chemical

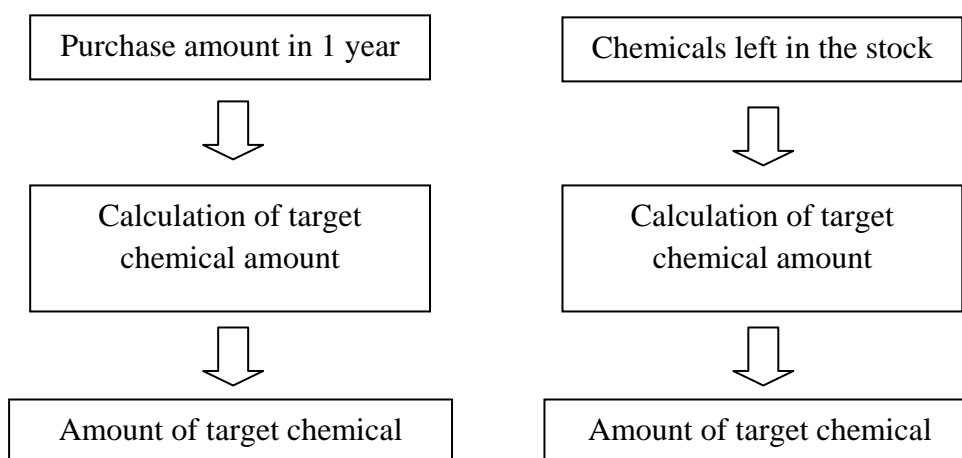


Figure 3.2 Estimation of possessed annual amount of target chemical

Air concentration of target chemicals from direct measurement is used in the estimation of emission data which is expressed in the unit of emission amount per time using the box model approach and ventilation engineering calculation. These data are used together with volume of laboratory to evaluate emission rate or volatilization rate of such chemical due to laboratory activities. The principle of calculation is summarized as shown in Figure 3.2.

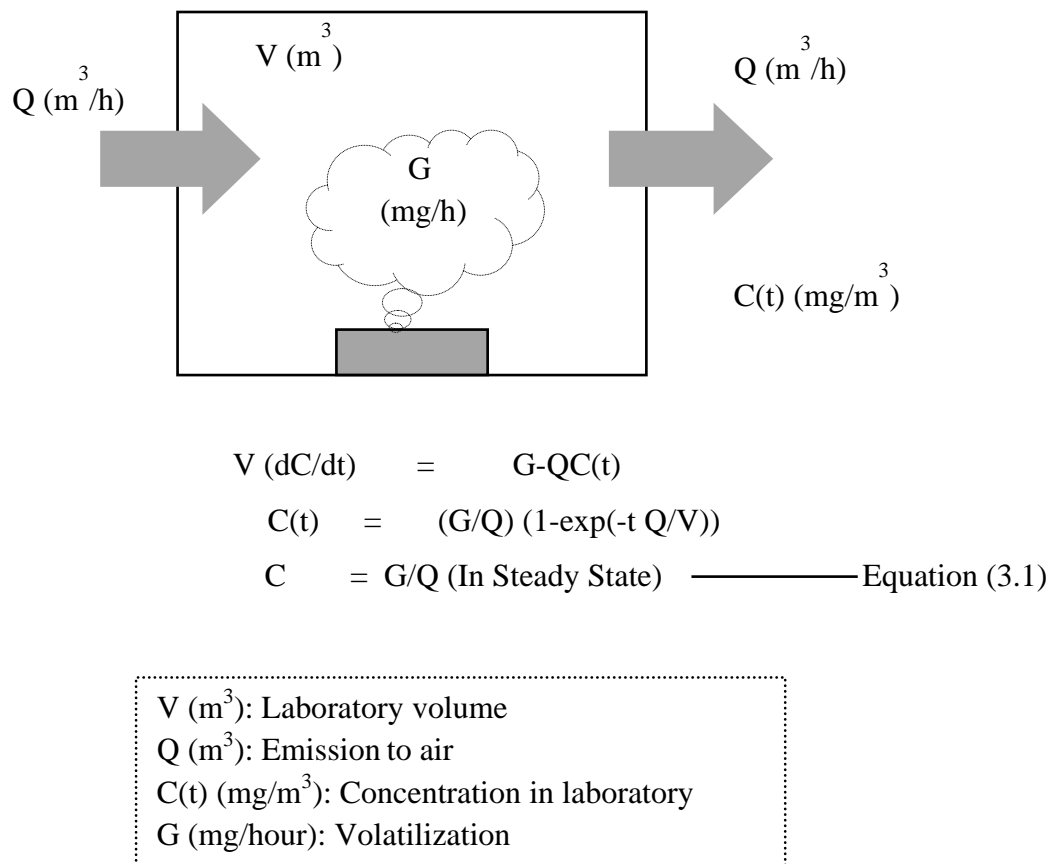


Figure 3.3 Equation for estimation of average concentration (Nomura et al., 2006)

To measure amount of target chemicals in wastewater

$$R_{\text{water}} = C_w \times V_w \times 10^{-6} \quad \text{————— Equation (3.2)}$$

$R_{\text{water}} =$ the amount of target chemicals that are released into the wastewater. (kg/year).

C_w = Concentrations of the target chemicals in the wastewater.
(mg/m³)

V_w = Volume of wastewater (m³/year)

3.4 Sampling and analytical methods

Sampling and analysis methodology of selected chemical in each pilot chemical laboratory is summarized in Table 3.2. Details are as followed.

Table 3.2 Summary of sampling and analysis of selected chemicals

Pilot laboratory	Selected chemical	Sampling	Analysis
Rayong Wittayakom school	Ethyl acetate	Adsorption (charcoal tube)	GC-FID NIOSH 1457
Mahidol University	Ethyl acetate	Adsorption (charcoal tube)	GC-FID NIOSH 1457
PTT-Global Chemical Co.,Ltd.	Isopropyl alcohol	Adsorption (charcoal tube)	GC-FID NIOSH 1400
	Toluene		GC-FID NIOSH 1501

At Rayong Wittayakom school, ethyl acetate is selected for estimation of emission. This chemical is used as a solvent in experimental laboratory of grade 11 student. Ethyl acetate was sampling by active method using adsorbed charcoal tube (SKC Anasorb® CSC, Coconut Charcoal catalog no.226-01) with flow rate 0.08 L/min in 60 minutes. The adsorption samples were analyzed by GC-FID (NIOSH 1457).

At Mahidol University, ethyl acetate is selected for estimation of emission. This chemical is used as a solvent in experiment laboratory. Ethyl acetate was sampling by active method using adsorbed charcoal tube (SKC Anasorb® CSC, Coconut Charcoal catalog no.226-01) with flow rate 0.08 L/min in 60 minutes. The adsorption samples were analyzed by GC-FID (NIOSH 1457).

At PTT-Global Chemical Co.,Ltd. isopropyl alcohol and toluene are selected for estimation of emission. This chemical is used as a solvent in chemical extraction. Isopropyl alcohol and toluene were sampling by active method using adsorbed charcoal tube (SKC Anasorb® CSC, Coconut Charcoal catalog no.226-01) with flow rate 0.15 L/min in 60 minutes and 30 minutes respectively. The adsorption samples were analyzed by GC-FID (NIOSH 1457 and NIOSH 1501, respectively).

The sampling and analysis methodology of selected chemical in each chemical laboratory is shown in Appendix A.

3.5 Estimation of release and emission rate

Principle of estimation is based on the mass balance and direct measurement techniques. Annual possess of chemical substances are used as input data in mass balance calculation. Data are used to subtract with total possess amount to evaluate emission to other environment medias. Details area as summarized below.

Mass balance model:

$$\text{Input} = \text{Output} + \text{Waste}$$

Measured concentrations are used to calculate emission amount to air by using equation (1). As for emission amount to water, this amount is calculated by subtracting the total amount of chemical consumption with amount of target chemical used and emission to air as shown below.

$\text{Emission to water} = \text{Total amount} - \text{Total used} - \text{Emission to air}$ <p>(kg/year)</p>
--

Laboratory wastes were sent to disposal authorities. These transfer amounts is estimated by manifest for each selected chemical of each pilot laboratory.

3.5.1 Estimation of chemical release and emission rate

Results of the emission estimation of target chemical to air and water are expressed in the unit of emission amount per year (kg/year). These data are analyzed and reported in the format of appropriate emission rate with available activity data of

laboratory. Therefore, the emission rates are expressed in the unit of amount of target chemical emission per student per year (kg/student/year) taking into consideration the applicability of this emission rate for further analysis of other schools.

3.5.2 Ventilation calculation

Ventilation system is exchanging of indoor and outdoor air. Air change per hour is a measure of how many times the air within a defined space (normally a room or house) is replaced.

For example, 10 Air change means that total volume of air in the room are replaced 10 times in 1 hour or the total volume of air in the room is replaced every 6 minutes. Ventilation equation can be expressed as follows:

Equation (3.3)

$$\text{Ventilation rate (m}^3/\text{h)} = \text{Volume of the room (m}^3\text{)} \times \text{ACH (air change per hour)}$$

When:

ACH = air change per hour (m³/h)

3.5.3 Emission calculation

Average concentrations of chemicals measured in the laboratory are used together with ventilation data to calculate emission rate of substances to air environment. Average concentration (using either arithmetic mean or median) values are used as appropriate taking into consideration distribution profile of the measured data. The emission amounts of target chemicals to air and water are expressed in the unit of kg of substance to air/water per year. Emission calculation is expressed as follows:

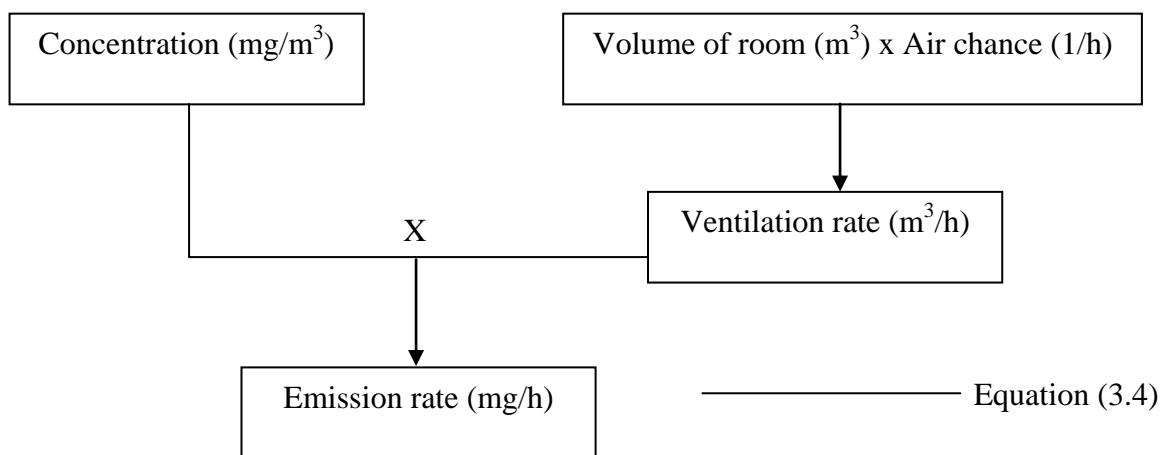


Figure 3.4 Calculation of emission rate

3.6 Experimental design of the study

The experimental design can be shows as a flow chart in Figure 3.5

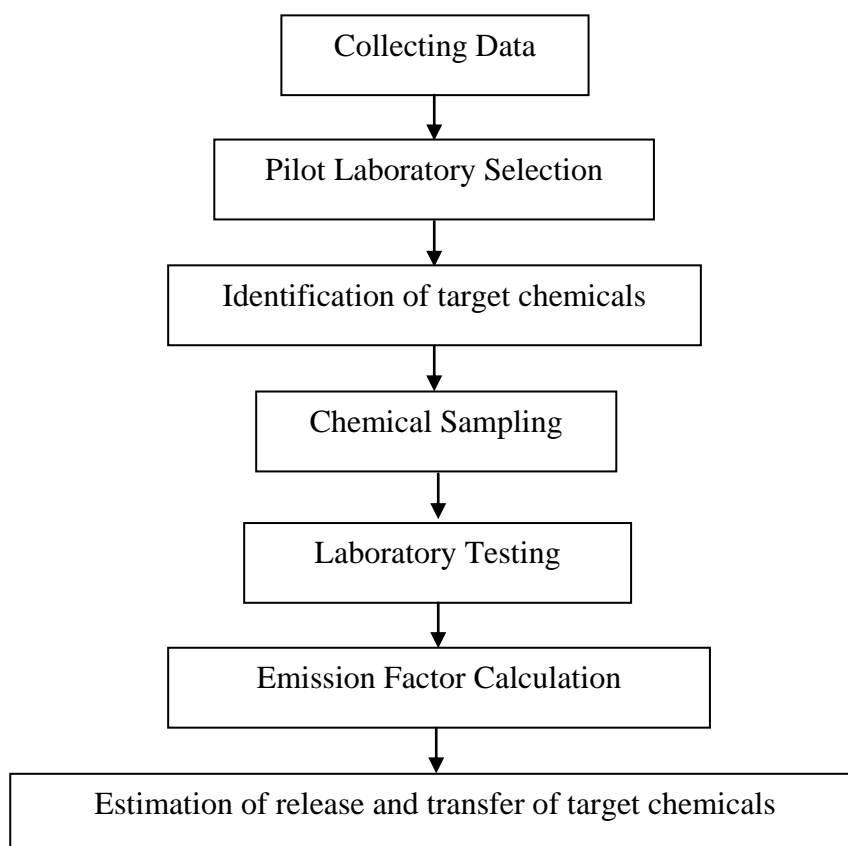


Figure 3.5 Flow chart of the experimental design

CHAPTER IV

RESULTS AND DISCUSSION

In this chapter, the measurement data and results of concentration and emission were presented. Details were as follows:

4.1 Data collection

Data amount of chemical substances from 107 PRTR's target chemical in sample laboratory were collected from inventory data per year. Summary of data was as shown in Table 4.1-4.3. Table 4.1 was amount of chemical using in Rayong Wittayakom school. Ten chemical substances were possessed in this laboratory. Table 4.2 showed twelve amount of chemical using in Central laboratory, Mahidol University. Twelve chemical substances were possessed in this laboratory. Table 4.3 presented amount of chemical using in PTT Global Chemical laboratory. There were 10 chemical substances, possessed in this laboratory.

Table 4.1 Amount of chemicals using in Rayong Wittayakom school laboratory

Chemicals in laboratory	Amount of chemical (L/year)	Amount of chemical (Kg/year)
1. Acetone	0.10	0.08
2. Ethyl acetate	2.25	2.01
3. Formaldehyde	0.15	0.16
4. Hexane	1.35	0.88
5. Methanol	11.75	9.30
6. Naphthalene	0.10	0.11
7. Nickels and its compounds	-	-
8. Toluene	0.90	0.80

Chemical in laboratory	Amount of chemical (L/year)	Amount of chemical (Kg/year)
9. Xylene	0.45	0.39
10. Zincs and its compounds	-	-

Ethyl acetate was chosen as target chemical in school laboratory since it was used during the study period.

Table 4.2 Amount of chemical using in Central laboratory, Mahidol University

Chemical in laboratory	Amount of chemical (L/year)	Amount of chemical (Kg/year)
1. Acetone	0.20	0.16
2. Benzene	0.75	0.66
3. Carbon disulfide	1.50	1.89
4. Formaldehyde	0.20	0.21
5. Hexane	2.25	1.47
6. Isopropyl alcohol	4.40	3.45
7. Methanol	3.00	2.38
8. Methylene chloride	0.20	0.27
9. Methyl ethyl ketone	0.75	0.60
10. Styrene	0.20	0.18
11. Toluene	1.60	1.39
12. Xylene	0.50	0.43

During the study period, there were no 107 PRTR chemicals used in Central laboratory. Therefore, ethyl acetate was chosen to be chemical sample in this laboratory. The merit of choosing this chemical was the acquired results could be used to compare with general practice of laboratory activity in school.

Table 4.3 Amount of chemical using in PTT Global Chemical laboratory

Chemical in laboratory	Amount of chemical (L/year)	Amount of chemical (Kilogram/year)
1. Acetone	25	19.78
2. Benzene	2.5	2.20
3. Formaldehyde	0.5	0.53
4. Hexane	142.5	93.31
5. Isopropyl alcohol	1,628	1,278
6. Methanol	480	380
7. Phosphoric Acid	10	18.85
8. Tetrachloroethylene	325	527.15
9. Toluene	325	281.45
10. Xylene	25	21.6

Isopropyl alcohol and toluene were chosen as target chemical substances in this study. Selection criteria were based on its highest consumption in this laboratory.

4.2 Concentration of chemical substance

Concentration of chemical substance was converted from ppm to mg/m³

1) Rayong Wittayakom school

Ethyl acetate: (CH₃COOC₂H₅) MW = 88

Table 4.4 Concentration of ethyl acetate in Rayong Wittayakom school (opened condition)

Number of sample	Concentration (ppm)	Concentration (mg/m ³)
No.1	1.227	4.42
No.2	0.045	0.16
No.3	0.047	0.17
No.4	<0.001	0.00
Arithmetic Mean	0.33	1.19
Standard deviation (S.D.)	0.60	2.16
Median (med)	0.047	0.17

Average concentration of ethyl acetate in Rayong Wittayakom school (opened condition) was 1.19 mg/m³. This value was used in the next stage to calculate for emission rate.

Table 4.5 Concentration of ethyl acetate in Rayong Wittayakom school (closed condition)

Number of sample	Concentration (ppm)	Concentration (mg/m ³)
No.1	6.956	25.04
No.2	7.853	28.26
No.3	1.080	3.89
No.4	1.877	6.76
Arithmetic Mean	4.44	15.99
Standard deviation (S.D.)	3.46	12.44
Median (med)	3.95	15.90

Average concentration of ethyl acetate in Rayong Wittayakom school (closed condition) was 15.99 mg/m³. This value was used in the next stage to calculate for emission rate.

2) Central laboratory, Mahidol University

Ethyl acetate: ($\text{CH}_3\text{COOC}_2\text{H}_5$) MW= 88**Table 4.6** Concentration of ethyl acetate in Central laboratory, Mahidol University

Number of sample	Concentration (ppm)	Concentration (mg/m^3)
No.1	0.110	0.40
No.2	0.370	1.33
No.3	1.481	5.33
No.4	1.346	4.84
No.5	0.170	0.61
No.6	<0.001	0.00
No.7	0.485	1.75
No.8	0.175	0.63
No.9	2.047	7.37
No.10	0.072	0.26
No.11	1.252	4.50
No.12	1.521	5.47
Arithmetic Mean	0.752	2.71
Standard deviation (S.D.)	0.72	2.60
Median	0.43	1.54

Average concentration of ethyl acetate in Central laboratory was $2.71 \text{ mg}/\text{m}^3$.

This value was used in the next stage to calculate for emission rate.

3) PTT Global Chemical Co.,Ltd.

Isopropyl alcohol: $\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$ MW= 60

Table 4.7 Concentration of isopropyl alcohol in PTT Global Chemical Co.,Ltd.

Number of sample	Concentration (ppm)	Concentration (mg/m³)
No.1	<0.001	0.00
No.2	<0.001	0.00
No.3	0.875	2.15
No.4	<0.001	0.00
No.5	<0.001	0.00
No.6	<0.001	0.00
No.7	<0.001	0.00
No.8	<0.001	0.00
No.9	<0.001	0.00
No.10	<0.001	0.00
No.11	<0.001	0.00
No.12	<0.001	0.00
No.13	<0.001	0.00
No.14	<0.001	0.00
Arithmetic Mean	0.0625	0.15
Standard deviation (S.D.)	0.23	0.57
Median	0	0

Average concentration of isopropyl alcohol in PTT Global Chemical Co.,Ltd. was 0.15 mg/m³. This value was used in the next stage to calculate for emission rate.

Toluene: $C_6H_5CH_3$ MW= 92

Table 4.8 Concentration of toluene in PTT Global Chemical Co.,Ltd.

Number of sample	Concentration (ppm)	Concentration (mg/m^3)
No.1	2.35	8.84
No.2	<0.001	0.00
No.3	2.18	8.20
No.4	<0.001	0.00
No.5	4.58	17.23
No.6	4.81	18.10
Arithmetic Mean	2.32	8.73
Standard deviation (S.D.)	2.10	7.91
Median	2.27	8.52

Average concentration of toluene in PTT Global Chemical Co.,Ltd. was 8.73 mg/m^3 . This value was used in the next stage to calculate for emission rate.

4.3 Development of emission factor

Results from direct measurement of chemical concentrations were used to calculate for emission rate. These calculated values were used to develop emission factor of chemical, released to environment from laboratory activity.

Calculation of ethyl acetate emission rate from Rayong Wittayakom school

1) Open room condition

Ventilation rate calculation

- Dimension of laboratory: Width 8 m, Length 12 m, Height 3 m
- Door (1): 1.50 x 2.00 m
- Windows (30): 30 x 1.20 x 1.00 m
- Volume of the room = $8 \times 12 \times 3 = 288 \text{ m}^3$
- Air change for open room (ACH) = 20/h

$$\begin{aligned} \text{Ventilation rate} &= \text{Volume of the room} \times \text{ACH} \\ &= 288 \text{ m}^3 \times 20/\text{h} = 5,760 \text{ m}^3/\text{h} \end{aligned}$$

$$\text{From } Q = C \times V$$

$$\text{- } C = \text{concentration of ethyl acetate} = 1.19 \text{ mg/m}^3$$

$$\text{- } V = \text{ventilation volume} = 5,760 \text{ m}^3/\text{h}$$

$$\begin{aligned} \text{Therefore; } Q &= 1.19 \text{ mg/m}^3 \times 5,760 \text{ m}^3/\text{h} \\ &= 6,854.4 \text{ mg/h} \quad (\text{release to air}) \end{aligned}$$

$$\text{Total annual consumption} = 2.25 \text{ L}$$

$$\text{Amount of use in the lab} = 20 \text{ mL}$$

$$\text{Amount of actual use in the lab} = 10 \text{ mL}$$

$$\text{Excess amount} = 10 \text{ mL}$$

Calculation of ethyl acetate emission from Rayong Witthayakom school

- Amount of ethyl acetate release to air

$$\text{- } 20 \text{ mL of ethyl acetate will be released to air at about } 6,854.4 \text{ mg}$$

Total annual consumption of ethyl acetate was 2.25 L. Therefore, the annual release to air was estimated as:

$$= (6,854.4 \text{ mg} / 2,250 \text{ mL}) / 20 \text{ mL} = 0.77 \text{ kg/year}$$

$$2.25 \text{ L of ethyl acetate} = 2.01 \text{ kg.}$$

Therefore 1000 kg of ethyl acetate used in the lab will be released to air

$$= (0.77 \text{ kg/h} \times 1000 \text{ kg}) / 2.01 \text{ kg}$$

$$= 383.09 \text{ kg release to air} / 1000 \text{ kg of ethyl acetate use in the lab}$$

- Release of ethyl acetate to water

$$= \text{Amount of use in the lab} - \text{amount of actual use} - \text{emission to air}$$

$$= 17.89 \text{ g} - 8.945 \text{ g} - 6.854 \text{ g} = 2.091 \text{ g/h}$$

Annual release of ethyl acetate to water

$$= \text{annual amount of use} - \text{annual amount of actual use} - \text{annual emission to air}$$

$$= 2.01 \text{ kg} - 1.005 \text{ kg} - 0.77 \text{ kg}$$

$$= 0.24 \text{ kg/year}$$

- Transfer of ethyl acetate to waste

Since the wastes in the school were drained to the sewage system, it was estimated that transfer of ethyl acetate to waste was negligible.

Calculation of emission factor in the unit of release amount to air per student per year

- Annual amount of ethyl acetate emission to air = 0.77 kg/year

- Number of student (grade 9-12) = 1,813 person

Therefore, emission factor in the unit of release amount to air per student per year

= Annual amount of ethyl acetate emission to air / Number of student (grade 9-12)

= (0.77 kg/year) / (1,813 person)

= 4.25×10^{-4} kg/person/year

Calculation of emission factor in the unit of release amount to water per student per year

- Annual amount of ethyl acetate emission to water = 0.77 kg/year

- Number of student (grade 9-12) = 1,813 person

Therefore, emission factor in the unit of release amount to water per student per year

= Annual amount of ethyl acetate emission to water / Number of student (grade 9-12)

= (0.19 kg/year) / (1,813 person)

= 1.05×10^{-4} kg/person/year

2) Closed room condition

Ventilation rate calculation

- Dimension of laboratory: 8 m x 12 m x 3 m
- Door (1): 1.50 x 2.00 m
- Windows (30): 30 x 1.20 x 1.00 m
- Volume of the room = $8 \times 12 \times 3 = 288 \text{ m}^3$
- Air change for windows or exterior doors on one side = 0.67/h

$$\begin{aligned} \text{Ventilation rate} &= \text{Volume of room} \times \text{ACH} \\ &= 288 \text{ m}^3 \times 0.67/\text{h} = 192.96 \text{ m}^3/\text{h} \end{aligned}$$

From: $Q = C \times V$

- $C = \text{concentration of ethyl acetate} = 15.99 \text{ mg/m}^3$

- $V = \text{ventilation rate} = 192.96 \text{ m}^3/\text{h}$

$$\begin{aligned} \text{Therefore; } Q &= 15.99 \text{ mg/m}^3 \times 192.96 \text{ m}^3/\text{h} \\ &= 3,085.43 \text{ mg/h} \quad (\text{release to air}) \end{aligned}$$

Total annual consumption = 2.25 L

Amount of use in the lab = 20 mL

Amount of actual use in the lab = 10 mL

Excess amount = 10 mL

Calculation of ethyl acetate emission from Rayong Witthayakom school

- Amount of ethyl acetate release to air

- 20 mL of ethyl acetate will be released to air at about 3,085.43 mg

Total annual consumption of ethyl acetate was 2.25 L. Therefore, the annual release to air was estimated as:

$$= (3,085.43 \text{ mg} / 2,250 \text{ mL}) / 20 \text{ mL} = 0.35 \text{ kg/year}$$

2.25 L of ethyl acetate = 2.01 kg.

Therefore 1000 kg of ethyl acetate used in the lab will be released to air

$$= (0.35 \text{ kg/h} \times 1000 \text{ kg}) / 2.01 \text{ kg}$$

$$= 174.13 \text{ kg release to air} / 1000 \text{ kg of ethyl acetate use in the lab}$$

- Release of ethyl acetate to water

$$= \text{Amount of use in the lab} - \text{amount of actual use} - \text{emission to air}$$

$$= 17.89 \text{ g} - 8.945 \text{ g} - 3.085 \text{ g} = 5.86 \text{ g/h}$$

Annual release of ethyl acetate to water

$$= \text{annual amount of use} - \text{annual amount of actual use} - \text{annual emission to air}$$

$$= 2.01 \text{ kg} - 1.05 \text{ kg} - 0.35 \text{ kg}$$

$$= 0.61 \text{ kg/year}$$

- Transfer of ethyl acetate to waste

Since the wastes in the school were drained to the water, it was estimated that transfer of ethyl acetate to waste was negligible.

Calculation of emission factor in the unit of release amount to air per student per year

- Annual amount of ethyl acetate emission to air = 0.35 kg/year
- Number of student (grade 9-12) = 1,813 person

Therefore, emission factor in the unit of release amount to air per student per year

$$\begin{aligned}
 &= \text{Annual amount of ethyl acetate emission to air} / \text{Number of student (grade 9-12)} \\
 &= (0.35 \text{ kg/year}) / (1,813 \text{ person}) \\
 &= 1.93 \times 10^{-4} \text{ kg/person/year}
 \end{aligned}$$

Calculation of emission factor in the unit of release amount to water per student per year

- Annual amount of ethyl acetate emission to water = 0.61 kg/year
- Number of student (grade 9-12) = 1,813 person

Therefore, emission factor in the unit of release amount to water per student per year

$$\begin{aligned}
 &= \text{Annual amount of ethyl acetate emission to water} / \text{Number of student (grade 9-12)} \\
 &= (0.61 \text{ kg/year}) / (1,813 \text{ person}) \\
 &= 3.36 \times 10^{-4} \text{ kg/person/year}
 \end{aligned}$$

Calculation of ethyl acetate emission rate at central laboratory, Mahidol University

Ventilation rate calculation

- Dimension of laboratory: 14 m x 16 m x 3 m
- Door (2): 2 x 1.80 x 2.00 m
- Windows (6): 6 x 1.50 x 0.70 m
- Volume of the room = 14 x 16 x 3 = 672 m³
- Dimension of fume hood: 1.0 m x 1.0 m x 2.50 m = 2.50 m³

- Volumetric flow rate of hood = $1.215 \text{ m}^3/\text{s} = 72.9 \text{ m}^3/\text{min}$
 - Air change = 1,765/h (see calculation in appendix C)
- Ventilation rate = Volume of hood x ACH
 = $2.5 \text{ m}^3 \times 1,765/\text{h} = 4,412.5 \text{ m}^3/\text{h}$

From: $Q = C \times V$

- C = concentration of ethyl acetate = $2.71 \text{ mg}/\text{m}^3$
- V = ventilation rate = $4,412.5 \text{ m}^3/\text{h}$

Therefore: $Q = 2.71 \text{ mg}/\text{m}^3 \times 4,412.5 \text{ m}^3/\text{h}$
 $= 11,957.88 \text{ mg}/\text{h}$ (release to air)

Amount of chemical use = 30 mL

Amount of actual use = 30 mL

Excess amount = 0 mL

Calculation of ethyl acetate emission from Mahidol University

- Amount of ethyl acetate release to air

- 30 mL of ethyl acetate (26.84 g) will be released to air at about 11,957.88 mg

In this study, amount of ethyl acetate, used in laboratory was about 180 mL (161.01 g). Therefore, release of ethyl acetate was:

$$= (11.958 \text{ g} \times 161.01 \text{ g}) / 26.84 \text{ g}$$

$$= 71.73 \text{ g}$$

This value can be express as = 445.53 kg of ethyl acetate release to air/ 1000 kg of ethyl acetate used in the laboratory

- Amount of ethyl acetate release to water

No chemical used in the laboratory were drained to the water. All of them were collected in a bottle/container and was sent for laboratory waste disposal. Therefore, release to water was negligible in this case.

- Transfer of ethyl acetate to waste

Assumption for calculation of chemical transfer to waste

- For each batch of the laboratory activity, about 1.5 times of an actual chemical use will be brought out from its container (worst case condition).

Therefore, the consumption amount of isopropyl alcohol when working with actual amount of use as 30 mL = 30 mL x 1.5 = 45 mL

$$\text{Annual consumption of ethyl acetate} = 1.5 \times 161.01 \text{ g/year} = 241.52 \text{ g/year}$$

Annual amount of transfer of ethyl acetate to waste

$$= \text{Annual amount of consumption} - \text{Annual amount of use} - \text{release to air}$$

$$= 241.52 \text{ g} - 161.01 \text{ g} - 11.96 \text{ g}$$

$$= 68.55 \text{ g/year}$$

- For each batch of the laboratory activity, about 10% or 1.1 times of an actual chemical use will be brought out from its container (normal activity condition).

Therefore, the consumption amount of isopropyl alcohol when working with actual amount of use as 30 mL = 30 mL x 1.1 = 33 mL

$$\text{Annual consumption of ethyl acetate} = 1.2 \times 161.01 \text{ g/year} = 177.11 \text{ g/year}$$

Annual amount of transfer of ethyl acetate to waste

$$= \text{Annual amount of consumption} - \text{Annual amount of use} - \text{release to air}$$

$$= 177.11 \text{ g} - 161.01 \text{ g} - 11.96 \text{ g}$$

$$= 4.14 \text{ g/year}$$

Table 4.9 Comparison of ethyl acetate transfer to waste

Assumption	Amount transfer to waste (g/year)
1.1 times of an actual use (normal activity condition)	4.14
1.5 times of an actual use (worst case condition)	68.55

These data revealed that the amount of pollutant, transferred to waste was depended on a good practice of the laboratory.

Calculation of isopropyl alcohol emission rate from PTT Global Chemical Co.,Ltd.

Ventilation rate calculation

- Dimension of fume hood: 2.0 m x 1.0 m x 2.35 m = 4.70 m³
- Volumetric flow rate of hood = 2.0 x 1.0 x 2.35 = 1.786 m³/s = 107.2 m³/min
- Air change = 1,364/h

$$\begin{aligned} \text{Ventilation rate} &= \text{volume of hood} \times \text{ACH} \\ &= 4.70 \text{ m}^3 \times 1,364/\text{h} = 6,410.8 \text{ m}^3/\text{h} \end{aligned}$$

From: $Q = C \times V$

- C = concentration of isopropyl alcohol = 2.15 mg/m³
- V = ventilation rate = 6,410.8 m³/h

$$\begin{aligned} \text{Therefore: } Q &= 2.15 \text{ mg/m}^3 \times 6,410.8 \text{ m}^3/\text{h} \\ &= 13,783.22 \text{ mg/h} \quad (\text{release to air}) \end{aligned}$$

Total annual consumption	=	1,628 L
Amount of use in the lab	=	400 mL
Amount of actual use in the lab	=	400 mL
Excess amount	=	0 mL

Calculation of isopropyl alcohol emission from PTT Global Chemical Co.,Ltd.

- Amount of isopropyl alcohol release to air

- 400 mL of isopropyl alcohol will be released to air at about 13,783.22 mg

Total annual consumption of isopropyl alcohol was 1628 L. Therefore, the annual release to air was estimated as:

$$= (13,783.22 \text{ mg/h} \times 1,628 \text{ L}) / 400 \text{ mL} = 56.10 \text{ kg/year}$$

The fume hood of this laboratory is equipped with activated carbon adsorber. The VOCs controlling efficiency of this equipment is estimated as 95% removal of VOCs concentration (Wei-Wei Qiu (2002) "Prevention of Significant Air Quality Deterioration"). Therefore, emission of isopropyl alcohol to air was estimated as:

$$\begin{aligned} &= 56.10 \text{ kg/year} - ((95/100) \times 56.10 \text{ kg/year}) \\ &= 2.81 \text{ kg/year} \end{aligned}$$

The emission factor can be calculated as

= 2.20 kg of isopropyl alcohol release to air/1000 kg of isopropyl alcohol use in the lab

- Amount of isopropyl alcohol release to water

No chemical used in the laboratory are drained to the water. All of them were collected in a bottle/container and was sent for laboratory waste disposal. Therefore, release to water was negligible in this case.

- Transfer of isopropyl alcohol to waste

Assumption for calculation of chemical transfer to waste

- For each batch of the laboratory activity, about 1.5 times of an actual chemical use will be brought out from its container (worst case condition).

Therefore, the consumption amount of isopropyl alcohol when working with actual amount of use as 400 mL = 400 mL x 1.5 = 600 mL

Annual consumption of isopropyl alcohol = 1.5 x 1,278 kg/year = 1,917 kg/year

Transfer of isopropyl alcohol to waste

= Annual consumption amount – annual amount of actual use – annual amount of air emission

$$= 1,917 \text{ kg/year} - 1,278 \text{ kg/year} - 56.10 \text{ kg/year}$$

$$= 582.9 \text{ kg/year}$$

- For each batch of the laboratory activity, about 10% or 1.1 times of an actual chemical use will be brought out from its container (normal activity condition).

Therefore, the consumption amount of isopropyl alcohol when working with actual amount of use as 400 mL = 400 mL x 1.1 = 440 mL

Annual consumption of isopropyl alcohol = 1.1 x 1,278 kg/year = 1,405.8 kg/year

Transfer of isopropyl alcohol to waste

= Annual consumption amount – annual amount of actual use – annual amount of air emission

$$= 1,405.8 \text{ kg/year} - 1,278 \text{ kg/year} - 56.10 \text{ kg/year}$$

$$= 71.7 \text{ kg/year}$$

Table 4.10 Comparison of isopropyl alcohol transfer to waste

Assumption	Amount transfer to waste (kg/year)
1.1 times of an actual use (normal activity condition)	71.7
1.5 times of an actual use (worst case condition)	582.9

These data revealed that the amount of pollutant, transferred to waste was depended on a good practice of the laboratory.

Calculation of toluene emission rate from PTT Global Chemical Co.,Ltd.

Ventilation rate calculation

- Dimension of fume hood: $2.0 \times 1.0 \times 2.35 = 4.70 \text{ m}^3$
- Volumetric flow rate of hood: $1.786 \text{ m}^3/\text{s} = 107.2 \text{ m}^3/\text{min}$
- Air change = 1364/h

$$\begin{aligned} \text{Ventilation rate} &= \text{Volume of hood} \times \text{ACH} \\ &= 4.70 \text{ m}^3 \times 1,364/\text{h} = 6,410.8 \text{ m}^3/\text{h} \end{aligned}$$

From: $Q = C \times V$

- C = concentration of toluene = $8.73 \text{ mg}/\text{m}^3$
- V = ventilation rate = $6,410.8 \text{ m}^3/\text{h}$

$$\begin{aligned} \text{Therefore: } Q &= 8.73 \text{ mg}/\text{m}^3 \times 6,410.8 \text{ m}^3/\text{h} \\ &= 55,966.28 \text{ mg}/\text{h} \quad (\text{release to air}) \end{aligned}$$

$$\begin{aligned} \text{Total annual consumption} &= 325 \text{ L} \\ \text{Amount of use in the lab} &= 300 \text{ mL} \\ \text{Amount of actual use in the lab} &= 300 \text{ mL} \\ \text{Excess amount} &= 0 \text{ mL} \end{aligned}$$

Calculation of toluene emission from PTT Global Chemical Co.,Ltd.

- Amount of toluene release to air

- 300 mL of isopropyl alcohol will be released to air at about 55.97 g

Total annual consumption of toluene was 325 L. Therefore, the annual release to air was estimated as:

$$= (55.97 \text{ g} \times 325 \text{ L}) / 300 \text{ mL} = 60.63 \text{ kg/year}$$

The fume hood of this laboratory is equipped with activated carbon adsorber. The VOCs controlling efficiency of this equipment is estimated as 95% removal of VOCs concentration (Wei-Wei Qiu (2002) "Prevention of Significant Air Quality Deterioration"). Therefore, emission of toluene to air was estimated as:

$$= 60.63 \text{ kg/year} - ((95/100) \times 60.63 \text{ kg/year})$$

$$= 3.032 \text{ kg/year}$$

The emission factor can be calculated as

$$= 10.77 \text{ kg of toluene release to air/1000 kg of toluene use in the lab}$$

- Amount of toluene release to water

No chemical used in the laboratory are drained to the water. All of them will be collected in a bottle/container and be sent for laboratory waste disposal. Therefore, release to water was negligible in this case.

- Transfer of toluene to waste

Assumption for calculation of chemical transfer to waste

- For each batch of the laboratory activity, about 1.5 times of an actual chemical use will be brought out from its container (worst case condition).

Therefore, the consumption amount of toluene when working with actual amount of use as 300 mL = 300 mL x 1.5 = 450 mL

$$\text{Annual consumption of toluene} = 1.5 \times 281.45 \text{ kg/year} = 422.175 \text{ kg/year}$$

Transfer of toluene to waste

= Annual consumption amount – annual amount of actual use – annual amount of air emission

$$= 422.175 \text{ kg/year} - 281.45 \text{ kg/year} - 60.63 \text{ kg/year}$$

$$= 80.10 \text{ kg/year}$$

- For each batch of the laboratory activity, about 10% or 1.1 times of an actual chemical use will be brought out from its container (normal activity condition).

Therefore, the consumption amount of toluene when working with actual amount of use as 300 mL = 300 mL x 1.1 = 330 mL

$$\text{Annual consumption of toluene} = 1.1 \times 281.45 \text{ kg/year} = 309.60 \text{ kg/year}$$

Transfer of toluene to waste

= Annual consumption amount – annual amount of actual use – annual amount of air emission

$$= 309.60 \text{ kg/year} - 281.45 \text{ kg/year} - 60.63 \text{ kg/year}$$

$$= 4.48 \text{ kg/year}$$

Table 4.11 Comparison of toluene transfer to waste

Assumption	Amount transfer to waste (kg/year)
1.1 times of an actual use (normal activity condition)	4.48
1.5 times of an actual use (worst case condition)	80.10

These data revealed that the amount of pollutant, transferred to waste was depended on a good practice of the laboratory.

4.4 Emission factor of chemical from laboratory

Emission factor developed from direct measurement of concentration from each laboratory were different because of different characteristics of the laboratory and amount of usage in analytical activity. At Rayong Wittayakom school laboratory, the chemical experiments were carried out in two different conditions (opened and closed area). The emission factors of ethyl acetate in an opened and closed area were 382.9 kg/1000 kg usage and 172.44 kg/1000 kg usage, respectively. The emission factor of ethyl acetate, emitted from Mahidol University laboratory from direct measurement was calculated as 445.61 kg/1000 kg usage. As for PTT Global Chemical laboratory, measurements of target chemicals (isopropyl alcohol and toluene) were also carried out in a chemical fume hood. The emission factors of isopropyl alcohol and toluene of commercial laboratory were 2.2 kg/1000 kg usage and 10.77 kg/1000 kg usage, respectively. Results of emission factors from each laboratory were as summarized in Table 4.12.

Table 4.12 Emission factor of chemical from laboratory

Laboratory	Chemical	Emission factor (kg/1000 kg usage)	Remark
Rayong Wittayakom school	Ethyl acetate	383.09	Opened area
		174.13	Closed area
Mahidol University	Ethyl acetate	445.53	Fume hood
PTT Global Chemical Co.,Ltd.	Isopropyl alcohol	2.20	Fume hood + carbon adsorption
	Toluene	10.77	

4.5 Release estimation by engineering calculation

Input data: air temperature of laboratory, annual amount of chemical used, analytical times, molecular weight, the Antoine's constant

Where:

- P = vapor pressure of substance
 A, B, C = Antoine's constant (from Table 4.13)
 T = temperature (Celsius)

Example: Acetone; air temperature 30 °C, amount of use 100 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{acetone}} &= \exp A - (B/(T+C)) \\ &= \exp (7.11714 - (1210.595 / (30+229.664))) \\ &= 285.089 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{acetone}} = 1(P_{\text{ethyl acetate}}) = 285.089 \text{ mmHg}$$

$$\begin{aligned} V \text{ (ft}^3\text{)} &= 100 \text{ mL} \times 35.3147/10^6 \\ &= 3.53 \times 10^{-3} \text{ ft}^3 \end{aligned}$$

$$\text{From ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned}
 \text{Moles of acetone } n &= PV/RT \\
 &= (285.089 \times 3.53 \times 10^{-3}) / (998.9 \times 303) \\
 &= 3.33 \times 10^{-6} \text{ lb-moles} \\
 \text{Acetone weight} &= 3.33 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 1.51 \times 10^{-3} \text{ g-mole} \times 58.08 \text{ g/g-mole} \\
 &= 0.087 \text{ g/h/batch}
 \end{aligned}$$

Therefore, every 100 mL of acetone used, about 0.084 g/h/batch of acetone will be released to air.

Table 4.13 Constant of the Antoine's equation of PRTR target chemicals (107 substances)

Chemical substance	Temperature (°C)	A	B	C
Acetaldehyde	-0.2 to 34.4	8.00552	1600.017	291.809
Acetone	-12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	20.0 to 70.0	5.65204	648.629	154.683
Benzene	14.5 to 80.9	6.89272	1203.531	219.888
Carbon disulfide	3.6 to 79.0	6.94279	1169.11	241.593
Chloroform	-10.4 to 60.3	6.95465	1170.966	226.232
Cyclohexanol	93.7 to 160.7	6.25530	912.866	109.126
Dichloroethane 1,2-	-30.8 to 99.4	7.02530	1271.254	222.927
Ethyl acetate	15.6 to 75.8	7.10179	1244.951	217.881
Ethylene glycol	50.0 to 200.0	8.09083	2088.936	203.454
Ethylene oxide	0.3 to 31.8	8.69016	2005.779	334.765
Formaldehyde	-109.4 to 22.3	7.19578	970.595	244.124
Formic acid	37.4 to 100.7	7.58178	1699.173	260.713
Hexane	13.0 to 69.5	6.88555	1175.817	224.867
Isopropyl alcohol	22.3 to 89.3	7.74021	1359.517	197.527

Chemical substance	Temperature (°C)	A	B	C
Methanol	14.9 to 83.7	8.08097	1582.271	239.726
Methyl acetate	1.8 to 55.8	7.06524	1157.630	219.726
Methyl ethyl ketone	42.8 to 88.4	7.06356	1261.339	221.969
Methyl isobutyl ketone	21.7 to 116.2	6.67272	1168.408	191.944
Methyl methacrylate	39.2 to 89.2	8.40919	2050.467	274.369
Methylene chloride	-40.0 to 40	7.40916	1325.938	252.616
Naphthalene	80.3 to 179.5	7.03358	1756.328	204.842
Styrene	29.9 to 128.3	7.06623	1507.434	214.985
Trichloroethylene	17.8 to 86.5	6.51827	1018.603	192.731
Tetrachloroethylene	14.1 to 76.0	7.02000	1415.490	221.010
Pentane, n-	13.3 to 36.8	6.84471	1060.793	231.541
Phenol	107.2 to 181.8	7.13301	1516.790	174.954
Propionic acid	72.4 to 128.3	7.71423	1733.418	217.724
Toluene	22.9 to 111.5	6.95805	1346.773	219.693
Vinyl acetate	21.8 to 72.0	7.21010	1296.130	226.655
m-Xylene	59.2 to 140.0	7.00646	1460.183	214.827
o-Xylene	63.5 to 140.0	7.00154	1476.393	213.872
p-Xylene	58.3 to 139.3	6.98820	1451.792	215.111

Emission factors, calculated by using engineering calculation were presented in Table 4.14. Details of calculation in each laboratory were elaborated in Appendix D.

Table 4.14 Summary of emission factor of chemical using engineering calculation (unit kg of chemical/1000 kg used in the laboratory)

Chemical substance (kg/1000 kg using)	Rayong Wittayakom school	Mahidol University	PTT Global Chemical Co.,Ltd.
Acetone	1.09	0.90	0.91
Benzene	-	0.45	0.45
Carbon disulfide	-	1.17	-
Ethyl acetate	0.63	-	-
Formaldehyde	6.74	6.00	5.92
Hexane	1.31	1.07	1.07
Isopropyl alcohol	-	0.18	0.18
Methanol	0.35	0.28	0.28
Methylene chloride	-	1.46	-
Methyl ethyl ketone	-	0.48	-
Naphthalene	0.002	-	-
Styrene	-	0.04	-
Tetrachloroethylene	-	-	0.10
Toluene	0.20	0.16	0.16
Xylene	0.07	0.05	0.05

4.6 Emission Inventory of ethyl acetate for school for Rayong province

Emission amount of ethyl acetate of Rayong Wittayakom school (open room) = 0.77 kg/year

Emission amount of ethyl acetate of Rayong Wittayakom school (close room) = 0.35 kg/year

- Total number of high school student in Rayong Wittayakom school = 1,813 students

Emission factor of ethyl acetate in the unit of kg/student/year

$$= (0.77 \text{ kg/year}) / 1,813 \text{ students}$$

$$= 4.25 \times 10^{-4} \text{ kg/student/year} \dots\dots\dots (\text{case of open room})$$

$$= (0.35 \text{ kg/year}) / 1,813 \text{ students}$$

$$= 1.93 \times 10^{-4} \text{ kg/student/year} \dots\dots\dots (\text{case of close room})$$

Emission factor of ethyl acetate in the unit of kg/student/year in case of open room and close room were 4.25×10^{-4} kg/student/year and 1.93×10^{-4} kg/student/year, respectively.

Total number of high school student in each district of the province was as shown in Table 4.15. These data were used to multiply with emission factor to determine emission amount of chemicals to air from the school in Rayong province.

$$\text{Emission of ethyl acetate} = \text{Emission factor} \times \text{number of student}$$

Table 4.15 Number of student in Rayong province

District	Number of student (grade 9-12)
Muang Rayong	7,005
Ban Chang	1,030
Klang	2,082
Wang Chan	655
Ban Khai	1,089
Puak Daeng	883
Khao Chamao	495
Nikom pattana	502
Total	13,741

Emission factor of the open room was used in this analysis. Emission amount of ethyl acetate in all districts Rayong province were 2.98, 0.44, 0.88, 0.28, 0.46, 0.38, 0.21 and 0.21 kg/year respectively. Total emission of ethyl acetate release to air was 5.84 kg/year. Results were as shown in Table 4.16.

Table 4.16 Emission of ethyl acetate release to air from school in Rayong province

District	Emission amount of ethyl acetate (kg/y)
Muang Rayong	2.98
Ban chang	0.44
Klang	0.88
Wang chan	0.28
Ban Khai	0.46
Puak Daeng	0.38
Kao chamao	0.21
Nikom pattana	0.21
Total	5.84

The highest emission amount of ethyl acetate was found in Muang Rayong due to the large number of high school student in this district (>50% of total number of student in Rayong province).

4.7 Emission Inventory of chemical substance using in laboratory

Emission factor of the open room was used in this analysis. Total emission of chemical substance release to air was 5.26 kg/year. Results were as shown in Table 4.17.

Table 4.17 Rayong Wittayakom school laboratory

Chemical substance	Amount of chemical (kg/year)	Emission Inventory (kg/year)
Acetone	0.08	0.03
Ethyl acetate	2.01	0.77
Formaldehyde	0.16	0.06
Hexane	0.88	0.34
Methanol	9.30	3.56
Naphthalene	0.11	0.04
Nickels and its compounds	-	-

Chemical substance	Amount of chemical (kg/year)	Emission Inventory (kg/year)
Toluene	0.80	0.31
Xylene	0.39	0.15
Zincs and its compounds	-	-
Total	13.73	5.26

Remark: Emission factor used in the calculation was obtained from direct measurement of ethyl acetate emission.

Emission factor of ethyl acetate was used in this analysis. Total emission of chemical substance release to air was 5.81 kg/year. Results were as shown in Table 4.18.

Table 4.18 Central laboratory, Mahidol University

Chemical substance	Amount of chemical (kg/year)	Emission Inventory (kg/year)
Acetone	0.16	0.07
Benzene	0.66	0.29
Carbon disulfide	1.89	0.84
Formaldehyde	0.21	0.09
Hexane	1.47	0.65
Isopropyl alcohol	3.45	1.54
Methanol	2.38	1.06
Methylene chloride	0.27	0.12
Methyl ethyl ketone	0.60	0.26
Styrene	0.18	0.08
Toluene	1.39	0.62
Xylene	0.43	0.19
Total	13.09	5.81

Remark: Emission factor used in the calculation was obtained from direct measurement of ethyl acetate emission.

Emission factor of toluene was used in this analysis. Total emission of chemical substance release to air was 17.29 kg/year. Results were as shown in Table 4.19.

Table 4.19 PTT Global Chemical laboratory

Chemical substance	Amount of chemical (kg/year)	Emission Inventory (kg/year)
Acetone	19.78	0.21
Benzene	2.20	0.02
Formaldehyde	0.53	0.006
Hexane	93.31	1.01
Isopropyl alcohol	1,278	2.81
Methanol	380	4.09
Phosphoric Acid	18.85	0.20
Tetrachloroethylene	527.15	5.68
Toluene	281.45	3.032
Xylene	21.6	0.23
Total	2,622.87	17.29

Remark: Emission factor used in the calculation was obtained from direct measurement of toluene emission.

However, the reporting criteria of PRTR required consumption of chemical more than 1000 kg/year to calculate and report in the system. Therefore only isopropyl alcohol at PTT Global Chemical Co.,Ltd. will be reported under reporting criteria of PRTR. The emission amount of isopropyl alcohol to air was 1,278 kg/year.

4.8 Application to use emission factor for chemical substances

Properties of chemical substance can be identified emission factor apply to use in other chemical substances.

Table 4.20 Chemical properties in Rayong Wittayakom school

Chemical substance	Vapor pressure (kPa@20°C)	Evaporation rate (Ether = 1)	Solubility (mg/L)	Health effect
Acetone	24.46	2.1	1.00×10^6	1
<i>Ethyl acetate</i>	9.8	2.9	8.3×10^3	1
Formaldehyde	0.2	-	-	4
Hexane	17.60	2.5	0.95×10^1	2
Methanol	13.02	3.5	Infinite	1
Naphthalene	0.006	<1	3.10×10^1	2
Nickels and its compounds	-	-	-	-
Toluene	3.8	6.1	5.26×10^2	2
Xylene	0.9	13.5	1.75×10^2	2
Zincs and its compounds	-	-	-	-

Source: (USEPA, 1995)

Chemical substance in Rayong Wittayakom school can be classified into three groups by considering their evaporation rate properties. Substances having evaporation rate less than 1 were put in group 1, Group 2 consisted of substances which their evaporation rates were about 1-5. Substances having evaporation rate more than 5 were put in group 3. Results were as shown in Table 4.21.

Table 4.21 Group of chemical substances in Rayong Wittayakom school

Group 1	Group 2	Group 3
Naphthalene	Acetone	Toluene
	<i>Ethyl acetate</i>	Xylene
	Formaldehyde	
	Hexane	
	Methanol	

Therefore, emission rate of ethyl acetate can be applied to other chemicals when their emission rates are unavailable, particularly with the chemical substances in group 2.

Table 4.22 Chemical properties in central laboratory, Mahidol University

Chemical substance	Vapor pressure (kPa@20°C)	Evaporation rate (Ether = 1)	Solubility (mg/L)	Health effect
Acetone	24.46	2.1	1.00×10^6	1
Benzene	10	5.1	1.75×10^3	2
Carbon disulfide	40	22.6	1.19×10^3	3
<i>Ethyl acetate</i>	9.8	2.9	8.3×10^3	1
Formaldehyde	0.2	-	4.0×10^6	4
Hexane	17.60	2.5	0.95×10^1	2
Isopropyl alcohol	4.4	11	Infinite	1
Methanol	13.02	3.5	Infinite	1
Methylene chloride	47	0.8	1.30×10^4	2
Methyl ethyl ketone	10.3	2.7	0.24×10^1	1
Styrene	0.6	0.49	3.10×10^2	2
Toluene	3.8	6.1	5.26×10^2	2
Xylene	0.9	13.5	1.75×10^2	2

Source: (USEPA, 1995)

Chemical substance in Mahidol University can be classified into four groups by considering their evaporation rate properties. Substances having evaporation rate less than 1 were put in group 1, Group 2 consisted of substances which their evaporation rates were about 1-5. Substances having evaporation rate were about 5-10 were put in group 3. Group 4 consisted of substances which their evaporation rates more than 10. Results were as shown in Table 4.23.

Table 4.23 Group of chemical substances in Mahidol University

Group 1	Group 2	Group 3	Group 4
Methylene chloride	Acetone	Benzene	Carbon disulfide
Styrene	<i>Ethyl acetate</i>	Toluene	Isopropyl alcohol
	Hexane		Xylene
	Methanol		
	Methyl ethyl ketone		

Therefore, emission rate of ethyl acetate can be applied to other chemicals when their emission rates are unavailable, particularly with the chemical substances in group 2.

Table 4.24 Chemical properties in PTT-Global Chemical Co.,Ltd

Chemical substance	Vapor pressure (kPa@20°C)	Evaporation rate (Ether = 1)	Solubility (mg/L)	Health effect
Acetone	24.46	2.1	1.00×10^6	1
Benzene	10	5.1	1.75×10^3	2
Formaldehyde	0.2	-	4.0×10^6	4
Hexane	17.60	2.5	0.95×10^1	2
<i>Isopropyl alcohol</i>	<i>4.4</i>	<i>11</i>	<i>Infinite</i>	<i>1</i>
Methanol	13.02	3.5	Infinite	1
Phosphoric acid	0.004	-	-	3
Tetrachloroethylene	1.7	0.9	2.00×10^2	2
<i>Toluene</i>	<i>3.8</i>	<i>6.1</i>	5.26×10^2	2
Xylene	0.9	13.5	1.75×10^2	2

Source: (USEPA, 1995)

Chemical substance in PTT-Global Chemical Co.,Ltd. can be classified into four groups by considering their evaporation rate properties. Substances having evaporation rate less than 1 were put in group 1, Group 2 consisted of substances

which their evaporation rates were about 1-5. Substances having evaporation rate were about 5-10 were put in group 3. Group 4 consisted of substances which their evaporation rates more than 10. Results were as shown in Table 4.25.

Table 4.25 Group of chemical substances in PTT-Global Chemical Co.,Ltd

Group 1	Group 2	Group 3	Group 4
Tetrachloroethylene	Acetone	Benzene	<i>Isopropyl alcohol</i>
	Hexane	<i>Toluene</i>	Xylene
	Methanol		

Therefore, emission rate of isopropyl alcohol can be applied to other chemicals when their emission rates are unavailable, particularly with the chemical substances in group 4. Emission rate of toluene can be applied with the chemical substances in group 3.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

The overall result and findings from this study were summarized in this chapter. Conclusions with respect to the objectives of the study were presented.

5.1 Conclusions

In this study, emission factors of chemical compounds, listed under the Pollutant Release and Transfer Register (PRTR) of Thailand were estimated for chemical laboratory. Pilot laboratories selected in this study included school, university and commercial laboratories. Concentration of chemical in air environment was measured taking into account normal practice in each laboratory. The chemical concentration was collected by direct measurement method. Emission factors are expressed in the unit of amount of releasing to air per 1000 kg of chemical usage.

Results indicated that the highest emission factor was estimated at university laboratory (using ethyl acetate as target chemical). High emission rate was expected as result of using fume hood which will enhance the volatility rate of volatile organic compound. In school laboratory, emission rate was lower than university. Laboratory work in an open condition had higher emission rates of VOCs than those practice in a closed condition. The lowest emission rate of VOCs was observed at commercial laboratory. Good practice and using of appropriate VOCs control equipment were found to reduce emission of VOCs from this laboratory. Emission factors developed in this study were summerised in Table 5.1.

Table 5.1 Emission factor of chemical release to environment from laboratory

Laboratory	Chemicals	Release to air (kg/1000 kg usage)	Release to water (kg/1000 kg usage)	Release to waste (kg/1000 kg usage)	Remark
Rayong Wittayakom school	Ethyl acetate	383.09	119.40	0.00	Opened area
		174.13	328.36	0.00	Closed area
Mahidol University	Ethyl acetate	445.53	0.00	425.75	Fume hood
PTT Global Chemical Co.,Ltd.	Isopropyl alcohol	2.20	0.00	456.10	Fume hood + carbon adsorption
	Toluene	10.77	0.00	284.60	

Emission factor values from laboratory were difference because of different characteristics of the laboratory and amount of usage in analytical experiment. Opened area will have more emission to air than closed condition. In university, measurement of target chemical in the laboratory was conducted inside a chemical fume hood which is a general practice in university laboratory. As for commercial laboratory, measurements of target chemicals (isopropyl alcohol and toluene) were also carried out in a chemical fume hood. The difference of between emission factors of university and commercial laboratories were mainly as a result of having air treatment unit, installed together with the fume hood. The university laboratory doesn't have VOCs treatment device, installed with its fume hood. On the other hand, commercial laboratory has an activated carbon adsorption unit to treat an exhaust from the fume hood. It is estimated that about 95% of VOCs will be removed from this air pollution treatment device (USEPA AP-42).

Chemical substances were thought to be volatilized mainly through reduce pressure distillation. It was found that there was a loss of chemicals due to volatility. (Nomura et al., 2006) However the emission rate will be significantly decreased by installing VOCs treatment device at the fume hood and the management of chemical during experiment in laboratory. This emission factors can be applied to other laboratory when calculation of emission amount of PRTR chemicals are needed.

5.2 Limitation of this study

Limitations of this study were list as followed..

- Air sampling at the vent of laboratory could not be conducted due to a safety concern. Therefore, the control efficiency of C-adsorber from US.EPA was used in estimating the emission of chemicals to air for PTT Global Chemical Co.,Ltd. The minimum control efficiency (95% VOCs removal) was used in the calculation.

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APPENDICES

APPENDIX A

SAMPLING OF NIOSH METHOD

1. Method 1457 for ethyl acetate

Characteristics: CH₃COOC₂H₅ MW: 88.10 CAS: 141-78-6 RTECS: AH5425000

Sampling:

- Sampler: SOLID SORBENT TUBE (coconut shell charcoal, 100 mg/50 mg)
- Flow rate: 0.01 to 0.2 L/minute
- Volume: min 0.1 L @ 1400 mg/m³, max 10 L
- Shipment: refrigerated
- Sample stability: 6 days @ 5 °C
- Blank: 2 to 10 field blanks per set

Measurement:

- Technique: GAS CHROMATOGRAPHY, FID
- Analyte: ethyl acetate
- Extraction: 1 mL CS₂
- Injection volume: 1 µL
- Temperature injection: 250 °C
 - detector: 300 °C
 - column: 35 °C, 2 min; 10 °C/min to 150 °C
- Column: DB-Wax; 30 m, 0.32-mm ID, 1-µm film thickness
- Carrier gas: He, 1 mL/min
- Make up gas: N₂, 30 mL/min
- Calibration: standard solutions of ethyl acetate in CS₂
- Range: 1.5 to 1,000 µg per sample
- Estimated lod: 0.5 µg per sample
- Precision: 0.19 @ 40.5 to 810 µg per sample

Accuracy:

- Range studied: 704 to 2950 mg/m³ (6-L samples)
- Bias: -2.1%
- Overall precision: 0.058
- Accuracy: $\pm 11.8\%$

Sampling:

- 1) Calibrate each personal sampling pump with a representative sampler in line.
- 2) Break the ends of the sampler immediately before sampling. Attach sampler to personal sampling pump with flexible tubing.
- 3) Sample at an accurately known flow rate between 0.01 and 0.2 L/min for a total sample size of 0.2 to 10 L.
- 4) Cap the samplers with plastic (not rubber) caps and pack securely for shipment with bagged refrigerant.

Sample preparation:

- 5) Place the front and back sorbent sections of the sampler tube in separate vials. Discard the glass wool and foam plugs.
- 6) Add 1.0 mL CS₂ to each vial. Attach crimp cap to each vial. Note: Decane or other suitable internal standard at 0.1% v/v may be added at this step.
- 7) Allow to stand 30 min with occasional agitation.

Calibration and quality control:

- 8) Calibrate daily with at least six working standards over the range 8 to 1,000 µg analyte per sample.
 - a. Add known amounts of analyte to CS₂ in 10-mL volumetric flasks and dilute to the mark.
 - b. Analyze together with samples and blanks (steps 11 and 12).
 - c. Prepare calibration graph (peak area of analyte vs. mg ethyl acetate).
- 9) Determine desorption efficiency (DE) at least once for each lot of charcoal used for sampling in the calibration range (step 8). Prepare three tubes at each of five concentrations plus three media blanks.
- 10) Determine desorption efficiency (DE) for each lot of charcoal used for sampling in the calibration range (step 9).

- a. Remove and discard back sorbent section of a media blank sampler.
 - b. Inject a known amount of calibration stock solution directly onto front sorbent section with a microliter syringe.
 - c. Cap the tube. Allow to stand overnight.
 - d. Desorb (steps 5 through 7) and analyze together with working standards (steps 11 and 12).
 - e. Prepare a graph of DE vs. μg ethyl acetate recovered.
- 11) Analyze three quality control blind spikes and three analysis spikes to insure that the calibration graph and DE graph are in control.

Measurement:

- 12) Set gas chromatograph according to manufacturer's recommendations and to conditions given. Inject sample aliquot manually using solvent flush techniques or with autosampler. Note: If peak area is above the linear range of the working standards, dilute with CS_2 , reanalyze, and apply the appropriate dilution factor in calculations.
- 13) Measure peak area.

Calculations:

- 14) Determine the mass, μg (corrected for DE), of ethyl acetate found in the sample front (W_f) and back (W_b) sorbent sections, and in the average media blank front (B_f) and back (B_b) sorbent sections. Note: If $W_b > W_f/10$, report breakthrough and possible sample loss.
- 15) Calculate concentration, C , of ethyl acetate in the air volume sampled, V (L), at the sampling site.

$$C = (W_f + W_b - B_f - B_b) / V \quad \text{mg/m}^3$$

2. Method 1400 for isopropyl alcohol

Characteristics: $\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$ MW: 60.09 CAS: 67-63-0 RTECS: NT8050000

Sampling:

- Sampler: SOLID SORBENT TUBE (coconut shell charcoal, 100 mg/50 mg)
- Flow rate: 0.01 to 0.2 L/minute

- Volume: min 0.3 L, max 3 L
- Shipment: cooled
- Sample stability: unknown, store in freezer
- Blank: 2 to 10 field blanks per set

Measurement:

- Technique: GAS CHROMATOGRAPHY, FID
- Analyte: isopropyl alcohol
- Desorption: 1 mL 1% 2-butanol in CS₂
- Injection volume: 5 µL
- Temperature injection: 200 °C
 - detector: 250-300 °C
 - column: 65-70 °C,
- Column: glass 2 m x 4 mm ID, 0.2% Carbowax 1500 on 60/80 Carbopack

C or equivalent

- Carrier gas: N₂ or He, 30 mL/min
- Calibration: solutions of isopropyl alcohol in eluent (internal standard optional)

Accuracy: see evaluation of method

Sampling:

- 1) Calibrate each personal sampling pump with a representative sampler in line.
- 2) Break the ends of the sampler immediately before sampling. Attach sampler to personal sampling pump with flexible tubing.
- 3) Sample at an accurately known flow rate between 0.01 and 0.2 L/min for a total sample size of 0.3 to 3 L.
- 4) Cap the samplers with plastic (not rubber) caps and pack securely for shipment.

Sample preparation:

- 5) Place the front and back sorbent sections of the sampler tube in separate vials. Discard the glass wool and foam plugs.
- 6) Add 1.0 mL eluent to each vial. Attach crimp cap to each vial.
- 7) Allow to stand 30 min with occasional agitation.

Calibration and quality control:

- 8) Calibrate daily with at least six working standards over the range of the samples.
 - a. Add known amounts of analyte to eluent in 10-mL volumetric flasks and dilute to the mark.
 - b. Analyze together with samples and blanks (steps 11 and 12).
 - c. Prepare calibration graph (ratio of peak area of analyte of internal standard vs. mg isopropyl alcohol).
- 9) Determine desorption efficiency (DE) at least once for each lot of charcoal used for sampling in the calibration range (step 8). Prepare three tubes at each of five concentrations plus three media blanks.
 - a. Remove and discard back sorbent section of a media blank sampler.
 - b. Inject a known amount of calibration stock solution directly onto front sorbent section with a microliter syringe.
 - c. Cap the tube. Allow to stand overnight.
 - d. Desorb (steps 5 through 7) and analyze together with working standards (steps 11 and 12).
 - e. Prepare a graph of DE vs. μg ethyl acetate recovered.
- 10) Analyze three quality control blind spikes and three analysis spikes to insure that the calibration graph and DE graph are in control.

Measurement:

- 11) Set gas chromatograph according to manufacturer's recommendations and to conditions given. Inject sample aliquot manually using solvent flush techniques or with autosampler. Note: If peak area is above the linear range of the working standards, dilute with eluent, reanalyze, and apply the appropriate dilution factor in calculations.
- 12) Measure peak area. Divide the peak area of analyte by the peak area of internal standard on the same chromatogram.

Calculations:

- 13) Determine the mass, μg (corrected for DE), of ethyl acetate found in the sample front (W_f) and back (W_b) sorbent sections, and in the average media

blank front (B_f) and back (B_b) sorbent sections. Note: If $W_b > W_f/10$, report breakthrough and possible sample loss.

14) Calculate concentration, C , of ethyl acetate in the air volume sampled, V (L), at the sampling site.

$$C = (W_f + W_b - B_f - B_b) \times 10^3 / V \text{ mg/m}^3$$

3. Method 1501 for toluene

Characteristics: $C_6H_5CH_3$ MW: 92.14 CAS: 108-88-3 RTECS: XS5250000

Sampling:

- Sampler: SOLID SORBENT TUBE (coconut shell charcoal, 100 mg/50 mg)
- Flow rate: <0.20 L/min
- Volume: min 1 L, max 8 L
- Shipment: routine
- Sample stability: 30 days @ 5°C
- Blank: 10% of samples

Measurement:

- Technique: GAS CHROMATOGRAPHY, FID
- Analyte: toluene
- Desorption: 1 mL carbon disulfide; stand 30 min with agitation
- Injection volume : 1 μ L
- Temperature injection: 250°C
 - detector: 300 °C
 - column: 40 °C (10 min) to 230 °C (10°C/min)
- Column: capillary, fused silica 30 m x 0.32-mm ID; 1-m film 100% PEG

or equivalent

- Calibration: Solutions of analytes in CS_2
- Range: 0.024-4.51 mg
- Estimated lod: 0.7 μ g /sample
- Precision: 0.022

Accuracy:

- Range studied: 548 to 2190 mg/m³
- Bias: 1.6%
- Overall precision: 0.052
- Accuracy: $\pm 10.9\%$

Interferences: Under conditions of high humidity, the breakthrough volumes may be reduced. Other volatile organic compounds such as alcohols, ketones, ethers, and halogenated hydrocarbons are potential analytical interferences.

Sampling:

- 1) Calibrate each personal sampling pump with a representative sampler in line.
- 2) Break the ends of the sampler immediately before sampling. Attach sampler to personal sampling pump with flexible tubing.
- 3) Sample at an accurately known flow rate between 0.01 and 0.2 L/min for a total sample size of 1 to 8 L.
- 4) Cap the samplers with plastic (not rubber) caps and pack securely for shipment.

Sample preparation:

- 5) Place the front and back sorbent sections of the sampler tube in separate vials. Include the glass wool plug in the vial along with the front sorbent section.
- 6) Add 1.0 mL eluent to each vial. Attach crimp cap to each vial immediately.
- 7) Allow to stand 30 min with occasional agitation.

Calibration and quality control:

- 8) Calibrate daily with at least six working standards from below the LOD to 10 times the LOQ. If necessary, additional standards may be added to extend the calibration curve.
 - a. Add known amounts of analyte to eluent in 10-mL volumetric flasks and dilute to the mark. Prepare additional standards by serial dilution in 10-mL volumetric flasks.
 - b. Analyze together with samples and blanks (steps 11 through 12).
 - c. Prepare calibration graph (peak area of analyte vs. analyte per sample).

- 9) Determine desorption efficiency (DE) at least once for each lot of charcoal used for sampling in the calibration range (step 8).
 - a. Prepare three tubes at each of five concentrations plus three media blanks.
 - b. Inject a known amount of DE stock solution (5 to 25 μL) directly onto front sorbent section with a microliter syringe.
 - c. Allow the tubes to air equilibrate for several minutes, then cap the tube and allow to stand overnight.
 - d. Desorb (steps 5 through 7) and analyze together with working standards (steps 11 and 12).
 - e. Prepare a graph of DE vs. μg toluene recovered.
- 10) Analyze three quality control blind spikes and three analysis spikes to insure that the calibration graph and DE graph are in control.

Measurement:

- 11) Set gas chromatograph according to manufacturer's recommendations and to conditions given. Inject sample aliquot manually using solvent flush techniques or with autosampler. Note: If peak area is above the linear range of the working standards, dilute with eluent, reanalyze, and apply the appropriate dilution factor in calculations.
- 12) Measure peak area.

Calculations:

- 13) Determine the mass, μg (corrected for DE), of ethyl acetate found in the sample front (W_f) and back (W_b) sorbent sections, and in the average media blank front (B_f) and back (B_b) sorbent sections. Note: If $W_b > W_f/10$, report breakthrough and possible sample loss.
- 14) Calculate concentration, C, of ethyl acetate in the air volume sampled, V (L), at the sampling site.

$$C = (W_f + W_b - B_f - B_b) / V \quad \text{mg/m}^3$$

APPENDIX B

AIR CHANGE CALCULATION

Air change per hour is a measure of how many times the air within a defined space (normally a room or house) is replaced. (DOH, 2013)

Typical air changes per hour for well-insulated spaces:

- no windows or exterior doors - 0.33 ($1/h$)
- windows or exterior doors on one side - 0.67 ($1/h$)
- windows or exterior doors on two sides - 1 ($1/h$)
- window or exterior doors on three sides - 1.33 ($1/h$)

For example, 10 Air change means that total volume of air in the room will be replaced 10 times in 1 hour or the total volume of air in the room will be replaced every 6 minutes.

Air change for Mahidol University

- Volume of the hood = 2.5 m^3
 - Volumetric flow rate of hood = $1.215 \text{ m}^3/\text{s} = 72.9 \text{ m}^3/\text{min}$
 - $2.5/72.9 = 0.034$ min every 0.034 minute air in hood will be replaced
 - In 1 hour air in hood will be replaced = $60 \text{ minute}/0.034 \text{ minute} = 1,765$
- Air Change = 1,765/h

Air change for PTT-Global Chemical Co.,Ltd.

- Volume of the hood = 4.70 m^3
 - Volumetric flow rate of hood = $1.786 \text{ m}^3/\text{s} = 107.2 \text{ m}^3/\text{min}$
 - $4.70/107.2 = 0.034$ min every 0.044 minute air in hood will be replaced
 - In 1 hour air in hood will be replaced = $60 \text{ minute}/0.044 \text{ minute} = 1,364$
- Air Change = 1,364/h

APPENDIX C

PROPERTIES OF CHEMICAL SUBSTANCE

Table C-1 Properties of chemical substance use in pilot laboratories

Chemical substance	Molecular Weight (g/mol)	Density (g/mL)	Vapor pressure (kPa@20°C)
Acetone	58.08	0.791	24.46
Benzene	78.11	0.8786	10
Carbon disulfide	76.139	1.261	40
Dichloromethane	84.93	1.3266	47
Ethyl acetate	88.11	0.8945	9.8
Formaldehyde	30.03	1.067	1.52 (mmHg)
Hexane	86.18	0.6548	17.60
Isopropyl alcohol	60.10	0.785	4.4
Methanol	32.04	0.7918	13.02
Methyl ethyl ketone	72.11	0.8050	10.3
Naphthalene	128.17	1.14	0.05 (mmHg)
Phosphoric acid	97.995	1.885	0.0285 (mmHg)
Styrene	104.15	0.909	4.5 (mmHg)
Tetrachloroethylene	165.83	1.622	1.7

Chemical substance	Molecular Weight (g/mol)	Density (g/mL)	Vapor pressure (kPa@20°C)
Toluene	92.14	0.866	3.8
Xylene	106.16	0.864	0.9

APPENDIX D

ENGINEERING CALCULATION

- **Chemical at Rayong Wittayakom school**

1. Acetone

Air temperature = 30 °C, Amount of use = 100 mL/batch

Antoine equation: $\log_{10}P = A - (B/(T+C))$

$$\begin{aligned}
 P_{\text{acetone}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.11714 - (1210.595/ (30+229.664))) \\
 &= 285.089 \text{ mmHg}
 \end{aligned}$$

Raoult's Law: $p_{\text{acetone}} = 1(P_{\text{acetone}}) = 285.089 \text{ mmHg}$

$$\begin{aligned}
 V(\text{ft}^3) &= 100 \text{ mL} \times 35.3147/10^6 \\
 &= 3.53 \times 10^{-3} \text{ ft}^3
 \end{aligned}$$

Ideal gas law: $R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$

$$\begin{aligned}
 n(\text{acetone}) &= PV/RT \\
 &= (285.089 \times 3.53 \times 10^{-3}) / (998.9 \times 303) \\
 &= 3.33 \times 10^{-6} \text{ lb-moles}
 \end{aligned}$$

$$\begin{aligned}
 \text{Acetone weight} &= 3.33 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 1.51 \times 10^{-3} \text{ g-mole} \times 58.08 \text{ g/g-mole} \\
 &= 0.087 \text{ g}
 \end{aligned}$$

Every usage of 100 mL acetone, about 0.087g of acetone will be released to air.

Emission factor of acetone (release to air)

= 1.09 kg of acetone release to air/ 1000 kg of acetone used in the laboratory

2. Ethyl acetate

Air temperature = 30 °C, amount of use = 2.25 L/batch

Antoine equation: $\log_{10}P = A - (B/(T+C))$

$$\begin{aligned} P_{\text{ethyl acetate}} &= \exp A - (B/(T+C)) \\ &= \exp (7.10179 - (1244.951/ (30+217.881))) \\ &= 120.06 \text{ mmHg} \end{aligned}$$

Raoult's Law: $p_{\text{ethyl acetate}} = 1(P_{\text{ethyl acetate}}) = 120.06 \text{ mmHg}$

$$\begin{aligned} V(\text{ft}^3) &= 2250 \text{ mL} \times 35.3147/10^6 \\ &= 0.079 \text{ ft}^3 \end{aligned}$$

Ideal gas law: $R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$

$$\begin{aligned} n(\text{ethyl acetate}) &= PV/RT \\ &= (120.06 \times 0.079)/(998.9 \times 303) \\ &= 3.15 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Ethyl acetate weight} &= 3.15 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.014 \text{ g-mole} \times 88.11 \text{ g/g-mole} \\ &= 1.26 \text{ g} = 1.26 \times 10^{-3} \text{ kg} \end{aligned}$$

Every usage of 2.25 L ethyl acetate, about 1.26×10^{-3} kg of ethyl acetate will be released to air.

Emission factor of ethyl acetate (release to air)

= 0.63 kg of ethyl acetate release to air/ 1000 kg of ethyl acetate used in the laboratory

3. Formaldehyde

Air temperature = 30 °C, amount of use = 150 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{formaldehyde}} &= \exp A - (B/(T+C)) \\ &= \exp (7.19578 - (970.595/ (30+244.124))) \\ &= 4519.234 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{formaldehyde}} = 1(P_{\text{formaldehyde}}) = 4519.234 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 150 \text{ mL} \times 35.3147/10^6 \\ &= 5.297 \times 10^{-3} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{formaldehyde}) &= PV/RT \\ &= (4519.234 \times 5.297 \times 10^{-3}) / (998.9 \times 303) \\ &= 7.91 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Formaldehyde weight} &= 7.91 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.0359 \text{ g-mole} \times 30.03 \text{ g/g-mole} \\ &= 1.078 \text{ g} \end{aligned}$$

Every usage of 150 mL formaldehyde, about 1.08 g of ethyl acetate will be released to air.

Emission factor of formaldehyde (release to air)

= 6.74 kg of formaldehyde release to air/ 1000 kg of formaldehyde used in the laboratory

4. Hexane

Air temperature = 30 °C, amount of use 1.35 L/batch

$$\begin{aligned} \text{Antoine Equation: } \log_{10}P &= A - (B/(T+C)) \\ P_{\text{hexane}} &= \exp A - (B/(T+C)) \\ &= \exp (6.88555 - (1175.817 / (30+224.867))) \\ &= 187.1099 \text{ mmHg} \end{aligned}$$

$$\begin{aligned} \text{Raoult's Law: } p_{\text{hexane}} &= 1(P_{\text{hexane}}) = 187.1099 \text{ mmHg} \\ V(\text{ft}^3) &= 1350 \text{ mL} \times 35.3147/10^6 \\ &= 4.768 \times 10^{-2} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{hexane}) &= PV/RT \\ &= (187.1099 \times 4.768 \times 10^{-2}) / (998.9 \times 303) \\ &= 2.95 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Hexane weight} &= 2.95 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.0134 \text{ g-mole} \times 86.18 \text{ g/g-mole} \\ &= 1.152 \text{ g} \end{aligned}$$

Every usage of 1.35 L hexane, about 1.152 g of hexane will be released to air.

Emission factor of hexane (release to air)

= 1.31 kg of hexane release to air/ 1000 kg of hexane used in the laboratory

5. Methanol

Air temperature = 30 °C, amount of use = 11.75 L/batch

$$\begin{aligned} \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\ P_{\text{methanol}} &= \exp A - (B/(T+C)) \\ &= \exp (8.08097 - (1582.271 / (30+239.726))) \end{aligned}$$

$$\begin{aligned}
 &= 163.966 \text{ mmHg} \\
 \text{Raoult's Law: } p_{\text{methanol}} &= 1(P_{\text{methanol}}) = 163.966 \text{ mmHg} \\
 V(\text{ft}^3) &= 11750 \text{ mL} \times 35.3147/10^6 \\
 &= 0.41 \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K} \\
 n(\text{methanol}) &= PV/RT \\
 &= (163.966 \times 0.41)/(998.9 \times 303) \\
 &= 2.24 \times 10^{-4} \text{ lb-moles} \\
 \text{Methanol weight} &= 2.24 \times 10^{-4} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 0.102 \text{ g-mole} \times 32.05 \text{ g/g-mole} \\
 &= 3.268 \text{ g}
 \end{aligned}$$

Every usage of 11.75 L methanol, about 3.268 g of methanol will be released to air.

Emission factor of methanol (release to air)

= 351.40 g of methanol release to air/ 1000 kg of methanol used in the laboratory

6. Naphthalene

Air temperature = 30 °C, amount of use = 100 mL/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\
 P_{\text{naphthalene}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.03358 - (1756.328/ (30+204.842))) \\
 &= 0.35877 \text{ mmHg} \\
 \text{Raoult's Law: } p_{\text{naphthalene}} &= 1(P_{\text{naphthalene}}) = 0.35877 \text{ mmHg}
 \end{aligned}$$

$$\begin{aligned}
 V(\text{ft}^3) &= 100 \text{ mL} \times 35.3147/10^6 \\
 &= 3.531 \times 10^{-3} \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K} \\
 n(\text{naphthalene}) &= PV/RT \\
 &= (0.35877 \times 3.531 \times 10^{-3})/(998.9 \times 303) \\
 &= 4.186 \times 10^{-9} \text{ lb-moles} \\
 \text{Naphthalene weight} &= 4.186 \times 10^{-9} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 1.899 \times 10^{-6} \text{ g-mole} \times 128.17 \text{ g/g-mole} \\
 &= 2.43 \times 10^{-4} \text{ g/year}
 \end{aligned}$$

Every usage of 100 mL naphthalene, about 2.43×10^{-4} g of naphthalene will be released to air.

Emission factor of naphthalene (release to air)
 $= 2.21 \text{ g of naphthalene release to air} / 1000 \text{ kg of naphthalene used in the laboratory}$

7. Toluene

Air temperature = 30 °C, amount of use = 900 mL

$$\begin{aligned}
 \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\
 P_{\text{toluene}} &= \exp A - (B/(T+C)) \\
 &= \exp (6.95805 - (1346.773/ (30+219.693))) \\
 &= 36.672 \text{ mmHg} \\
 \text{Raoult's Law: } p_{\text{toluene}} &= 1(P_{\text{toluene}}) = 36.672 \text{ mmHg} \\
 V(\text{ft}^3) &= 900 \text{ mL} \times 35.3147/10^6 \\
 &= 3.178 \times 10^{-2} \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{toluene}) &= PV/RT \\ &= (36.672 \times 3.178 \times 10^{-2}) / (998.9 \times 303) \\ &= 3.85 \times 10^{-6} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Toluene weight} &= 3.85 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 1.747 \times 10^{-3} \text{ g-mole} \times 92.14 \text{ g/g-mole} \\ &= 0.1609 \text{ g} \end{aligned}$$

Every usage of 900 mL toluene, about 0.1609g of toluene will be released to air.

$$\begin{aligned} &\text{Emission factor of toluene (release to air)} \\ &= 201.13 \text{ g of toluene release to air/ 1000 kg of toluene used in the laboratory} \end{aligned}$$

8. Xylene

Air temperature = 30 °C, amount of use = 450 mL/batch

$$\begin{aligned} \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\ P_{\text{xylene}} &= \exp A - (B/(T+C)) \\ &= \exp (7.00646 - (1460.183 / (30+214.827))) \\ &= 11.023 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{xylene}} = 1(P_{\text{xylene}}) = 11.023 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 450 \text{ mL} \times 35.3147/10^6 \\ &= 1.589 \times 10^{-2} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$n(\text{xylene}) = PV/RT$$

$$\begin{aligned}
 &= (11.023 \times 1.589 \times 10^{-2}) / (998.9 \times 303) \\
 &= 5.885 \times 10^{-7} \text{ lb-moles} \\
 \text{Xylene weight} &= 5.89 \times 10^{-7} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 2.67 \times 10^{-4} \text{ g-mole} \times 106.16 \text{ g/g-mole} \\
 &= 0.0283 \text{ g}
 \end{aligned}$$

Every usage of 450 mL xylene, about 0.0283g of xylene will be released to air.

Emission factor of xylene (release to air)

$$= 72.56 \text{ g of xylene release to air} / 1000 \text{ kg of xylene used in the laboratory}$$

- **Chemicals at Mahidol University**

1. Acetone

Air temperature = 25 °C, amount of use = 200 mL/batch

Antoine equation: $\log_{10}P = A - (B/(T+C))$

$$\begin{aligned}
 P_{\text{acetone}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.11714 - (1210.595 / (30+229.664))) \\
 &= 230.911 \text{ mmHg}
 \end{aligned}$$

Raoult's Law: $p_{\text{acetone}} = 1(P_{\text{acetone}}) = 230.911 \text{ mmHg}$

$$\begin{aligned}
 V(\text{ft}^3) &= 200 \text{ mL} \times 35.3147/10^6 \\
 &= 7.06 \times 10^{-3} \text{ ft}^3
 \end{aligned}$$

Ideal gas law: $R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$

$$\begin{aligned}
 n(\text{acetone}) &= PV/RT \\
 &= (230.911 \times 7.06 \times 10^{-3}) / (998.9 \times 298) \\
 &= 5.47 \times 10^{-6} \text{ lb-moles}
 \end{aligned}$$

$$\begin{aligned}
 \text{Acetone weight} &= 3.33 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 2.49 \times 10^{-3} \text{ g-mole} \times 58.08 \text{ g/g-mole} \\
 &= 0.144 \text{ g}
 \end{aligned}$$

Every usage of 200 mL acetone, about 0.144g of acetone will be released to air.

$$\begin{aligned}
 &\text{Emission factor of acetone (release to air)} \\
 &= 900 \text{ g of acetone release to air} / 1000 \text{ kg of acetone used in the laboratory}
 \end{aligned}$$

2. Benzene

Air temperature = 25 °C, amount of use = 750 mL/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10} P &= A - (B/(T+C)) \\
 P_{\text{benzene}} &= \exp A - (B/(T+C)) \\
 &= \exp (6.89272 - (1203.531 / (25+219.888))) \\
 &= 95.083 \text{ mmHg}
 \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{benzene}} = 1(P_{\text{benzene}}) = 95.083 \text{ mmHg}$$

$$\begin{aligned}
 V(\text{ft}^3) &= 750 \text{ mL} \times 35.3147/10^6 \\
 &= 2.65 \times 10^{-2} \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned}
 n(\text{benzene}) &= PV/RT \\
 &= (95.083 \times 2.65 \times 10^{-2}) / (998.9 \times 298) \\
 &= 8.46 \times 10^{-6} \text{ lb-moles}
 \end{aligned}$$

$$\begin{aligned}
 \text{Benzene weight} &= 8.46 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 3.84 \times 10^{-3} \text{ g-mole} \times 78.11 \text{ g/g-mole}
 \end{aligned}$$

$$= 0.2997 \text{ g}$$

Every usage of 750 mL benzene, about 0.2997g of benzene will be released to air.

Emission factor of benzene (release to air)

$$= 454.09 \text{ g of benzene release to air/ 1000 kg of benzene used in the laboratory}$$

3. Carbon disulfide

Air temperature = 25 °C, amount of use = 1.50 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{Carbon disulfide}} &= \exp A - (B/(T+C)) \\ &= \exp (6.94279 - (1169.11 / (25+241.593))) \\ &= 360.924 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{Carbon disulfide}} = 1(P_{\text{carbon disulfide}}) = 360.924 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 1500 \text{ mL} \times 35.3147/10^6 \\ &= 0.053 \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{carbon disulfide}) &= PV/RT \\ &= (360.924 \times 0.053)/(998.9 \times 298) \\ &= 6.42 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Carbon disulfide weight} &= 6.42 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/1 kg} \\ &= 0.0291 \text{ g-mole} \times 76.139 \text{ g/g-mole} \\ &= 2.218 \text{ g} \end{aligned}$$

Every usage of 1.50 L carbon disulfide, about 2.218g of benzene will be released to air.

Emission factor of carbon disulfide (release to air)

= 1,173.5 g of carbon disulfide release to air/ 1000 kg of carbon disulfide used
in the laboratory

4. Formaldehyde

Air temperature = 25 °C, amount of use = 200 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{formaldehyde}} &= \exp A - (B/(T+C)) \\ &= \exp (7.19578 - (970.595/ (25+244.124))) \\ &= 3884.03 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{formaldehyde}} = 1(P_{\text{formaldehyde}}) = 3884.03 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 200 \text{ mL} \times 35.3147/10^6 \\ &= 7.06 \times 10^{-3} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{formaldehyde}) &= PV/RT \\ &= (3884.03 \times 5.297 \times 10^{-3}) / (998.9 \times 298) \\ &= 9.22 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Formaldehyde weight} &= 9.22 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/1 kg} \\ &= 0.0418 \text{ g-mole} \times 30.03 \text{ g/g-mole} \\ &= 1.26 \text{ g} \end{aligned}$$

Every usage of 200 mL formaldehyde, about 1.26g of formaldehyde will be released to air.

Emission factor of formaldehyde (release to air)

= 6,000 g of formaldehyde release to air/ 1000 kg of formaldehyde used in the laboratory

5. Hexane

Air temperature = 25 °C, amount of use = 2.25 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{hexane}} &= \exp A - (B/(T+C)) \\ &= \exp (6.88555 - (1175.817 / (25+224.867))) \\ &= 151.279 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{hexane}} = 1(P_{\text{hexane}}) = 151.279 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 2250 \text{ mL} \times 35.3147/10^6 \\ &= 7.95 \times 10^{-2} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{hexane}) &= PV/RT \\ &= (151.279 \times 7.95 \times 10^{-2}) / (998.9 \times 298) \\ &= 4.04 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Hexane weight} &= 4.04 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.0183 \text{ g-mole} \times 86.18 \text{ g/g-mole} \\ &= 1.579 \text{ g} \end{aligned}$$

Every usage of 2.25 L hexane, about 1.579 g of hexane will be released to air.

Emission factor of hexane (release to air)

= 1.07 kg of hexane release to air/ 1000 kg of hexane used in the laboratory

6. Isopropyl alcohol

Air temperature = 25 °C, amount of use = 4.40 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{isopropyl alcohol}} &= \exp A - (B/(T+C)) \\ &= \exp (7.74021 - (1359.517 / (25+197.527))) \\ &= 42.733 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{isopropyl alcohol}} = 1(P_{\text{isopropyl alcohol}}) = 42.733 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 4400 \text{ mL} \times 35.3147/10^6 \\ &= 0.155 \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{isopropyl alcohol}) &= PV/RT \\ &= (42.733 \times 0.155)/(998.9 \times 298) \\ &= 2.23 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Isopropyl alcohol weight} &= 2.23 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/1 kg} \\ &= 0.0101 \text{ g-mole} \times 60.10 \text{ g/g-mole} \\ &= 0.608 \text{ g} \end{aligned}$$

Every usage of 4.40 L isopropyl alcohol, about 0.608g of isopropyl alcohol will be released to air.

Emission factor of isopropyl alcohol (release to air)

= 176.23 g of isopropyl alcohol release to air/ 1000 kg of isopropyl alcohol used in the laboratory

7. Methanol

Air temperature = 25 °C, amount of use = 3.00 L/batch

$$\begin{aligned} \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\ P_{\text{methanol}} &= \exp A - (B/(T+C)) \\ &= \exp (8.08097 - (1582.271 / (25+239.726))) \\ &= 127.045 \text{ mmHg} \end{aligned}$$

$$\begin{aligned} \text{Raoult's Law: } p_{\text{methanol}} &= 1(P_{\text{methanol}}) = 127.045 \text{ mmHg} \\ V(\text{ft}^3) &= 3000 \text{ mL} \times 35.3147/10^6 \\ &= 0.11 \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{methanol}) &= PV/RT \\ &= (127.045 \times 0.011)/(998.9 \times 298) \\ &= 4.52 \times 10^{-5} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Methanol weight} &= 4.52 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 2.05 \times 10^{-2} \text{ g-mole} \times 32.05 \text{ g/g-mole} \\ &= 0.657 \text{ g} \end{aligned}$$

Every usage of 3.0 L methanol, about 0.657g of methanol will be released to air.

Emission factor of methanol (release to air)

= 276.05 g of methanol release to air/ 1000 kg of methanol used in the laboratory

8. Methylene chloride

Air temperature = 25 °C, amount of use = 200 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$P_{\text{methylene chloride}} = \exp A - (B/(T+C))$$

$$= \exp(7.40916 - (1325.938 / (25 + 252.616)))$$

$$= 429.538 \text{ mmHg}$$

$$\text{Raoult's Law: } p_{\text{methylene chloride}} = 1(P_{\text{methylene chloride}}) = 429.538 \text{ mmHg}$$

$$V(\text{ft}^3) = 200 \text{ mL} \times 35.3147/10^6$$

$$= 7.06 \times 10^{-3} \text{ ft}^3$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$n(\text{methylene chloride}) = PV/RT$$

$$= (429.538 \times 7.06 \times 10^{-3}) / (998.9 \times 298)$$

$$= 1.02 \times 10^{-5} \text{ lb-moles}$$

$$\text{Methylene chloride weight} = 1.02 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg}$$

$$= 4.62 \times 10^{-3} \text{ g-mole} \times 84.93 \text{ g/g-mole}$$

$$= 0.393 \text{ g}$$

Every usage of 200mL methylene chloride, about 0.393g of methylene chloride will be released to air.

Emission factor of methylene chloride (release to air)

= 1,456.56 g of methylene chloride release to air/ 1000 kg of methylene chloride used in the laboratory

9. Methyl ethyl ketone

Air temperature = 25 °C, amount of use = 750 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$P_{\text{methyl ethyl ketone}} = \exp A - (B/(T+C))$$

$$= \exp(7.06356 - (1261.339 / (25 + 221.969)))$$

$$= 90.424 \text{ mmHg}$$

$$\text{Raoult's Law: } p_{\text{methyl ethyl ketone}} = 1(P_{\text{methanol}}) = 90.424 \text{ mmHg}$$

$$V(\text{ft}^3) = 750 \text{ mL} \times 35.3147/10^6$$

$$= 0.026 \text{ ft}^3$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$n(\text{methyl ethyl ketone}) = PV/RT$$

$$= (90.424 \times 0.026)/(998.9 \times 298)$$

$$= 8.05 \times 10^{-6} \text{ lb-moles}$$

$$\text{Methyl ethyl ketone weight} = 8.05 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/1 kg}$$

$$= 3.65 \times 10^{-3} \text{ g-mole} \times 72.11 \text{ g/g-mole}$$

$$= 0.263 \text{ g/year}$$

Every usage of 750 mL methyl ethyl ketone, about 0.263g of methyl ethyl ketone will be released to air.

Emission factor of methyl ethyl ketone (release to air)

= 483.3 g of methyl ethyl ketone release to air/ 1000 kg of methyl ethyl ketone used in the laboratory

10. Styrene

Air temperature = 25 °C, amount of use = 200 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$P_{\text{styrene}} = \exp A - (B/(T+C))$$

$$= \exp (7.06623 - (1507.434/ (25+214.985)))$$

$$= 6.093 \text{ mmHg}$$

$$\text{Raoult's Law: } p_{\text{styrene}} = 1(P_{\text{styrene}}) = 6.093 \text{ mmHg}$$

$$V(\text{ft}^3) = 200 \text{ mL} \times 35.3147/10^6$$

$$\begin{aligned}
 &= 7.06 \times 10^{-3} \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K} \\
 n(\text{styrene}) &= PV/RT \\
 &= (6.093 \times 7.06 \times 10^{-3}) / (998.9 \times 298) \\
 &= 1.45 \times 10^{-7} \text{ lb-moles} \\
 \text{Styrene weight} &= 1.45 \times 10^{-7} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 6.56 \times 10^{-5} \text{ g-mole} \times 104.15 \text{ g/g-mole} \\
 &= 0.0068 \text{ g/year}
 \end{aligned}$$

Every usage of 200 mL styrene, about 0.0068g of styrene will be released to air.

Emission factor of styrene (release to air)
 = 37.78 g of styrene release to air/ 1000 kg of styrene used in the laboratory

11. Toluene

Air temperature = 25 °C, amount of use = 1.60 L/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10} P &= A - (B/(T+C)) \\
 P_{\text{toluene}} &= \exp A - (B/(T+C)) \\
 &= \exp (6.95805 - (1346.773 / (25+219.693))) \\
 &= 28.452 \text{ mmHg} \\
 \text{Raoult's Law: } p_{\text{toluene}} &= 1(P_{\text{toluene}}) = 28.452 \text{ mmHg} \\
 V(\text{ft}^3) &= 1600 \text{ mL} \times 35.3147/10^6 \\
 &= 5.65 \times 10^{-2} \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K}
 \end{aligned}$$

$$\begin{aligned}
 n(\text{toluene}) &= PV/RT \\
 &= (28.452 \times 5.65 \times 10^{-2}) / (998.9 \times 298) \\
 &= 5.40 \times 10^{-6} \text{ lb-moles} \\
 \text{Toluene weight} &= 5.40 \times 10^{-6} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 2.45 \times 10^{-3} \text{ g-mole} \times 92.14 \text{ g/g-mole} \\
 &= 0.226 \text{ g}
 \end{aligned}$$

Every usage of 1.60 L toluene, about 0.226 g of toluene will be released to air.

Emission factor of toluene (release to air)

= 162.59 g of toluene release to air/ 1000 kg of toluene used in the laboratory

12. Xylene

Air temperature = 25 °C, amount of use = 500 mL/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10} P &= A - (B/(T+C)) \\
 P_{\text{xylene}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.00646 - (1460.183 / (25+214.827))) \\
 &= 8.279 \text{ mmHg}
 \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{xylene}} = 1(P_{\text{xylene}}) = 8.279 \text{ mmHg}$$

$$\begin{aligned}
 V(\text{ft}^3) &= 500 \text{ mL} \times 35.3147 / 10^6 \\
 &= 1.766 \times 10^{-2} \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned}
 n(\text{xylene}) &= PV/RT \\
 &= (8.279 \text{ mmHg} \times 1.766 \times 10^{-2}) / (998.9 \times 303) \\
 &= 4.911 \times 10^{-7} \text{ lb-moles}
 \end{aligned}$$

$$\begin{aligned}
 \text{Xylene weight} &= 4.911 \times 10^{-7} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 2.23 \times 10^{-4} \text{ g-mole} \times 106.16 \text{ g/g-mole} \\
 &= 0.0237 \text{ g}
 \end{aligned}$$

Every usage of 500 mL xylene, about 0.0237g of xylene will be released to air.

Emission factor of xylene (release to air)

$$= 55.12 \text{ g of xylene release to air/ 1000 kg of xylene used in the laboratory}$$

- **Chemicals at PTT Global Chemical Co.,Ltd.**

1. Acetone

Air temperature = 25 °C, amount of use = 25 L/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10} P &= A - (B/(T+C)) \\
 P_{\text{acetone}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.11714 - (1210.595 / (25+229.664))) \\
 &= 230.911 \text{ mmHg}
 \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{acetone}} = 1(P_{\text{acetone}}) = 230.911 \text{ mmHg}$$

$$\begin{aligned}
 V(\text{ft}^3) &= 25000 \text{ mL} \times 35.3147/10^6 \\
 &= 0.883 \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned}
 n(\text{acetone}) &= PV/RT \\
 &= (230.911 \times 0.883)/(998.9 \times 298) \\
 &= 6.85 \times 10^{-4} \text{ lb-moles}
 \end{aligned}$$

$$\begin{aligned}
 \text{acetone weight} &= 6.85 \times 10^{-4} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 0.311 \text{ g-mole} \times 58.08 \text{ g/g-mole}
 \end{aligned}$$

$$= 18.04 \text{ g}$$

Every usage of 25 L acetone, about 18.04kg of acetone will be released to air.

Emission factor of acetone (release to air)

$$= 912.03 \text{ g of acetone release to air/ 1000 kg of acetone used in the laboratory}$$

2. Benzene

Air temperature = 25 °C, amount of use = 2.5 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$P_{\text{benzene}} = \exp A - (B/(T+C))$$

$$= \exp (6.89272 - (1203.531/ (25+219.888)))$$

$$= 95.083 \text{ mmHg}$$

$$\text{Raoult's Law: } p_{\text{benzene}} = 1(P_{\text{benzene}}) = 95.083 \text{ mmHg}$$

$$V(\text{ft}^3) = 2500 \text{ mL} \times 35.3147/10^6$$

$$= 0.088 \text{ ft}^3$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$n(\text{benzene}) = PV/RT$$

$$= (95.083 \times 0.088)/(998.9 \times 298)$$

$$= 2.82 \times 10^{-5} \text{ lb-moles}$$

$$\text{Benzene weight } wt = 2.82 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg}$$

$$= 0.0128 \text{ g-mole} \times 78.11 \text{ g/g-mole}$$

$$= 0.999 \text{ g}$$

Every usage of 2.5 L benzene, about 0.999g of benzene will be released to air.

Emission factor of benzene (release to air)

$$= 454.09 \text{ g of benzene release to air/ 1000 kg of benzene used in the laboratory}$$

3. Formaldehyde

Air temperature = 25 °C, amount of use = 500 mL/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{formaldehyde}} &= \exp A - (B/(T+C)) \\ &= \exp (7.19578 - (970.595/ (25+244.124))) \\ &= 3884.03 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{formaldehyde}} = 1(P_{\text{formaldehyde}}) = 3884.03 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 500 \text{ mL} \times 35.3147/10^6 \\ &= 1.77 \times 10^{-2} \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{formaldehyde}) &= PV/RT \\ &= (3884.03 \times 1.77 \times 10^{-2})/(998.9 \times 298) \\ &= 2.30 \times 10^{-4} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Formaldehyde weight} &= 2.30 \times 10^{-4} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.105 \text{ g-mole} \times 30.03 \text{ g/g-mole} \\ &= 3.138 \text{ g} \end{aligned}$$

Every usage of 500 mL formaldehyde, about 3.138g of formaldehyde will be released to air.

Emission factor of formaldehyde (release to air)

= 5,920.75 g of formaldehyde release to air/ 1000 kg of formaldehyde used in the laboratory

4. Hexane

Air temperature = 25 °C, amount of use = 142.5 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned}
 P_{\text{hexane}} &= \exp A - (B/(T+C)) \\
 &= \exp (6.88555 - (1175.817/ (25+224.867))) \\
 &= 151.279 \text{ mmHg} \\
 \text{Raoult's Law: } p_{\text{hexane}} &= 1(P_{\text{hexane}}) = 151.279 \text{ mmHg} \\
 V(\text{ft}^3) &= 142500 \text{ mL} \times 35.3147/10^6 \\
 &= 5.032 \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K} \\
 n(\text{hexane}) &= PV/RT \\
 &= (151.279 \times 5.032)/(998.9 \times 298) \\
 &= 2.56 \times 10^{-3} \text{ lb-moles} \\
 \text{Hexane weight} &= 2.56 \times 10^{-3} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 1.16 \text{ g-mole} \times 86.18 \text{ g/g-mole} \\
 &= 99.97 \text{ g}
 \end{aligned}$$

Every usage of 142.5 L hexane, about 99.97g of hexane will be released to air.
 Emission factor of hexane (release to air)
 = 1,071.37 g of hexane release to air/ 1000 kg of hexane used in the laboratory

5. Isopropyl alcohol

Air temperature = 25 °C, amount of use = 1628 L/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\
 P_{\text{isopropyl alcohol}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.74021 - (1359.517/ (25+197.527))) \\
 &= 42.733 \text{ mmHg}
 \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{isopropyl alcohol}} = 1(P_{\text{isopropyl alcohol}}) = 42.733 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 1628000 \text{ mL} \times 35.3147/10^6 \\ &= 57.49 \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{isopropyl alcohol}) &= PV/RT \\ &= (42.733 \times 57.49)/(998.9 \times 298) \\ &= 8.25 \times 10^{-3} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Isopropyl alcohol weight} &= 8.25 \times 10^{-3} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 3.74 \text{ g-mole} \times 60.10 \text{ g/g-mole} \\ &= 225 \text{ g} \end{aligned}$$

Every usage of 1,628 L Isopropyl alcohol, about 225g of Isopropyl alcohol will be released to air.

Emission factor of Isopropyl alcohol (release to air)

= 176.06 g of Isopropyl alcohol release to air/ 1000 kg of Isopropyl alcohol used in the laboratory

6. Methanol

Air temperature = 25 °C, amount of use = 480 L/batch

$$\text{Antoine equation: } \log_{10}P = A - (B/(T+C))$$

$$\begin{aligned} P_{\text{methanol}} &= \exp A - (B/(T+C)) \\ &= \exp (8.08097 - (1582.271/ (25+239.726))) \\ &= 127.04 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{methanol}} = 1(P_{\text{methanol}}) = 127.04 \text{ mmHg}$$

$$V(\text{ft}^3) = 480000 \text{ mL} \times 35.3147/10^6$$

$$\begin{aligned}
 &= 16.95 \text{ ft}^3 \\
 \text{Ideal gas law: } R &= 998.9 \text{ mmHg ft}^3/\text{lb-mole K} \\
 n(\text{methanol}) &= PV/RT \\
 &= (127.04 \times 16.95)/(998.9 \times 298) \\
 &= 7.23 \times 10^{-3} \text{ lb-moles} \\
 \text{Methanol weight} &= 7.23 \times 10^{-3} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 3.28 \text{ g-mole} \times 32.05 \text{ g/g-mole} \\
 &= 105 \text{ g}
 \end{aligned}$$

Every usage of 480 L methanol, about 105g of methanol will be released to air.

Emission factor of methanol (release to air)

= 276.32 g of methanol release to air/ 1000 kg of methanol used in the laboratory

7. Phosphoric acid: This calculation is not applicable to calculate release of this substance.

8. Tetrachloroethylene

Air temperature = 25 °C, amount of use = 325 L/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\
 P_{\text{tetrachloroethylene}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.02 - (1415.49/(25+221.01))) \\
 &= 18.459 \text{ mmHg}
 \end{aligned}$$

$$\begin{aligned}
 \text{Raoult's Law: } p_{\text{tetrachloroethylene}} &= 1(P_{\text{tetrachloroethylene}}) = 18.459 \text{ mmHg} \\
 V(\text{ft}^3) &= 325000 \text{ mL} \times 35.3147/10^6 \\
 &= 11.47 \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned} n(\text{tetrachloroethylene}) &= PV/RT \\ &= (163.966 \times 11.47)/(998.9 \times 298) \\ &= 7.12 \times 10^{-4} \text{ lb-moles} \end{aligned}$$

$$\begin{aligned} \text{Tetrachloroethylene weight} &= 7.12 \times 10^{-4} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\ &= 0.323 \text{ g-mole} \times 165.83 \text{ g/g-mole} \\ &= 53.54 \text{ g} \end{aligned}$$

Every usage of 325 L tetrachloroethylene, about 53.54g of tetrachloroethylene will be released to air.

Emission factor of tetrachloroethylene (release to air)
 = 101.57 g of tetrachloroethylene release to air/ 1000 kg of tetrachloroethylene used in the laboratory

9. Toluene

Air temperature = 25 °C, amount of use = 325 L/batch

$$\begin{aligned} \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\ P_{\text{toluene}} &= \exp A - (B/(T+C)) \\ &= \exp (6.95805 - (1346.773/ (25+219.693))) \\ &= 28.45 \text{ mmHg} \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{toluene}} = 1(P_{\text{toluene}}) = 28.45 \text{ mmHg}$$

$$\begin{aligned} V(\text{ft}^3) &= 325000 \text{ mL} \times 35.3147/10^6 \\ &= 11.48 \text{ ft}^3 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$n(\text{toluene}) = PV/RT$$

$$\begin{aligned}
 &= (28.45 \times 11.48)/(998.9 \times 298) \\
 &= 1.097 \times 10^{-3} \text{ lb-moles} \\
 \text{Toluene weight} &= 1.097 \times 10^{-3} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg} \\
 &= 0.498 \text{ g-mole} \times 92.14 \text{ g/g-mole} \\
 &= 45.85 \text{ g}
 \end{aligned}$$

Every usage of 325 L toluene, about 45.85g of toluene will be released to air.

Emission factor of toluene (release to air)

= 162.91 g of toluene release to air/ 1000 kg of toluene used in the laboratory

10. Xylene

Air temperature = 25 °C, amount of use = 25 L/batch

$$\begin{aligned}
 \text{Antoine equation: } \log_{10}P &= A - (B/(T+C)) \\
 P_{\text{xylene}} &= \exp A - (B/(T+C)) \\
 &= \exp (7.00646 - (1460.183/ (25+214.827))) \\
 &= 8.279 \text{ mmHg}
 \end{aligned}$$

$$\text{Raoult's Law: } p_{\text{xylene}} = 1(P_{\text{xylene}}) = 8.279 \text{ mmHg}$$

$$\begin{aligned}
 V(\text{ft}^3) &= 25000 \text{ mL} \times 35.3147/10^6 \\
 &= 0.883 \text{ ft}^3
 \end{aligned}$$

$$\text{Ideal gas law: } R = 998.9 \text{ mmHg ft}^3/\text{lb-mole K}$$

$$\begin{aligned}
 n(\text{xylene}) &= PV/RT \\
 &= (8.279 \times 0.883)/(998.9 \times 298) \\
 &= 2.46 \times 10^{-5} \text{ lb-moles}
 \end{aligned}$$

$$\text{Xylene weight} = 2.46 \times 10^{-5} \text{ lb-moles} \times 0.45359237 \text{ kg/lb} \times 10^3 \text{ g/kg}$$

$$= 0.011 \text{ g-mole} \times 106.16 \text{ g/g-mole}$$

$$= 1.18 \text{ g}$$

Every usage of 25 L xylene, about 1.8g of xylene will be released to air.

Emission factor of xylene (release to air)

= 54.63 g of xylene release to air/ 1000 kg of xylene used in the laboratory

APPENDIX E

CONVERSION FACTOR CALCULATION

1. Liter to kilogram

$$= \text{Volume} \times \text{Density}$$

2. mmHg to kPa

$$= (\text{mmHg} \times 133.322) / 1000$$

3. ppm to mg/m³

$$= (\text{MW} / 24.45) \times \text{ppm}$$

4. mean

$$\bar{x} = \frac{\sum X_i}{n}$$

Where $\sum X_i$ = sum of all data values

n = number of data items in sample

5. standard deviation

$$\text{S.D.} = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$$

Where \sum = sum of

x_i = each value in the data set

\bar{x} = mean of all value in the data set

N = number of value in the data set

APPENDIX F

SAMPLING ACTIVITY AT SELECTION LABORATORY



Figure F-1 Sampling activity at Rayong Witthayakom school

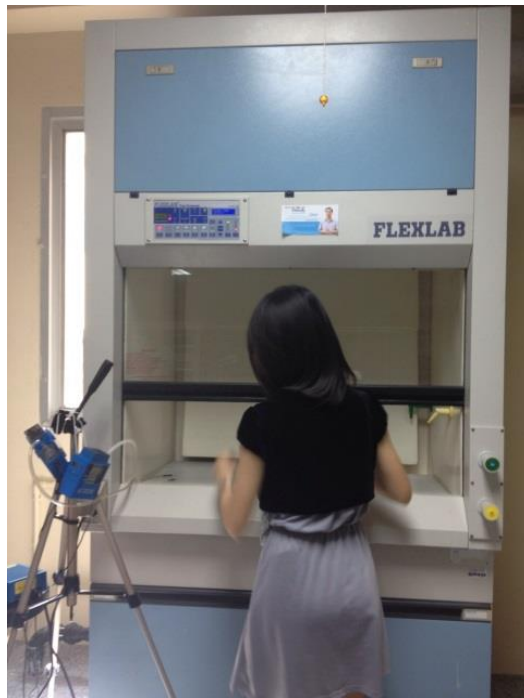


Figure F-2 Sampling activity at Central laboratory, Mahidol University



Figure F-3 Sampling activity at PTT Global Chemical Co.,Ltd.

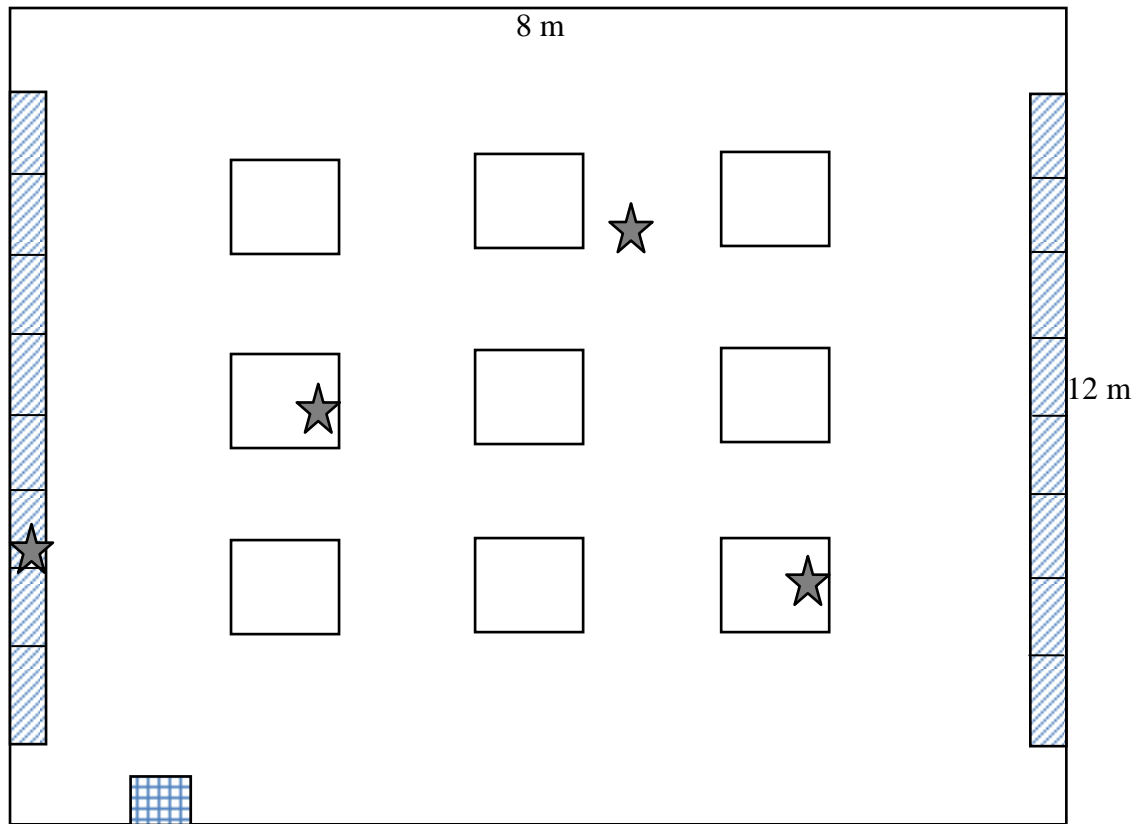






Figure F-4 Diagram of Rayong Wittayakom laboratory (Opened room)

-  Window
-  Door
-  Bench
-  Sampling point

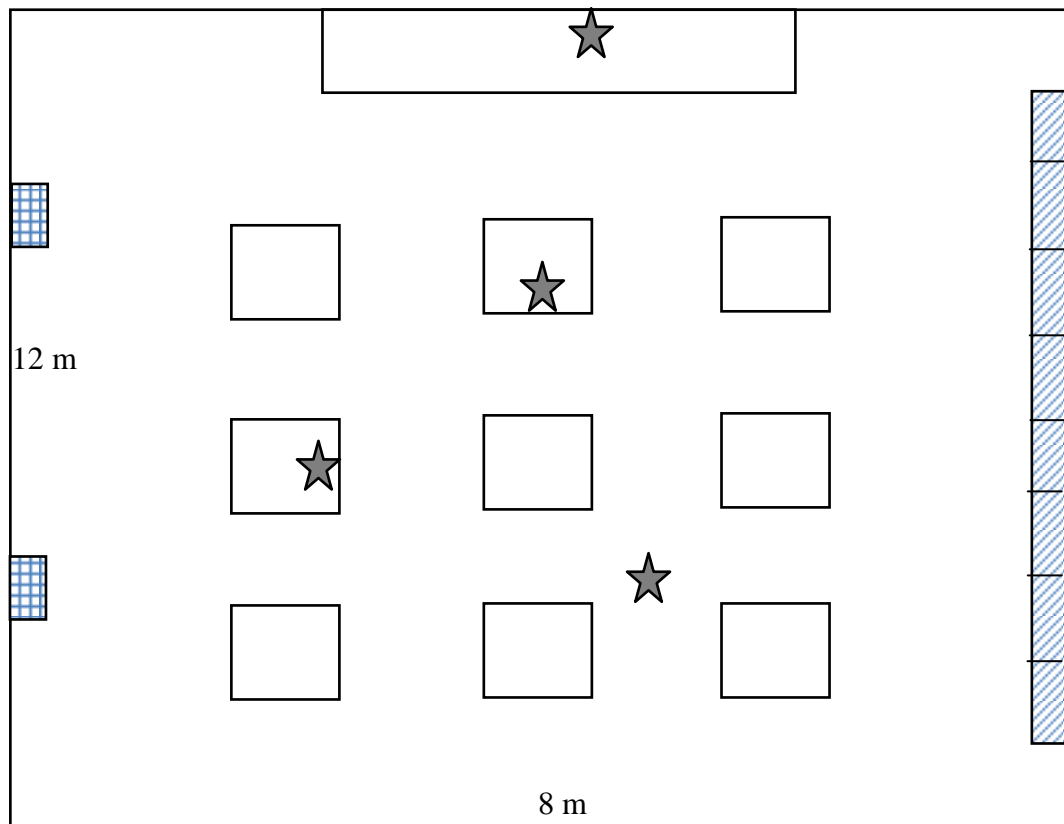
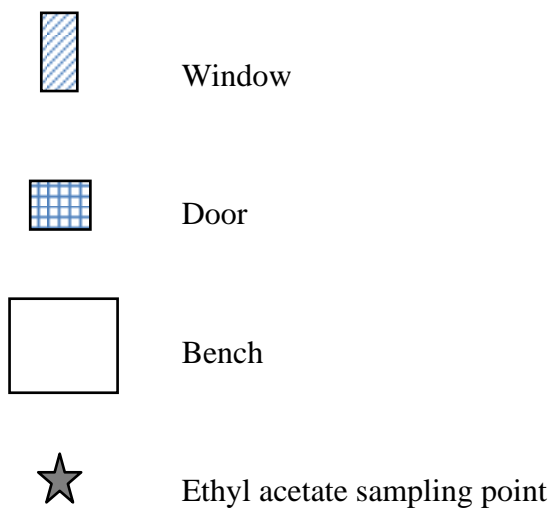


Figure F-5 Diagram of Rayong Wittayakom laboratory (Closed room)



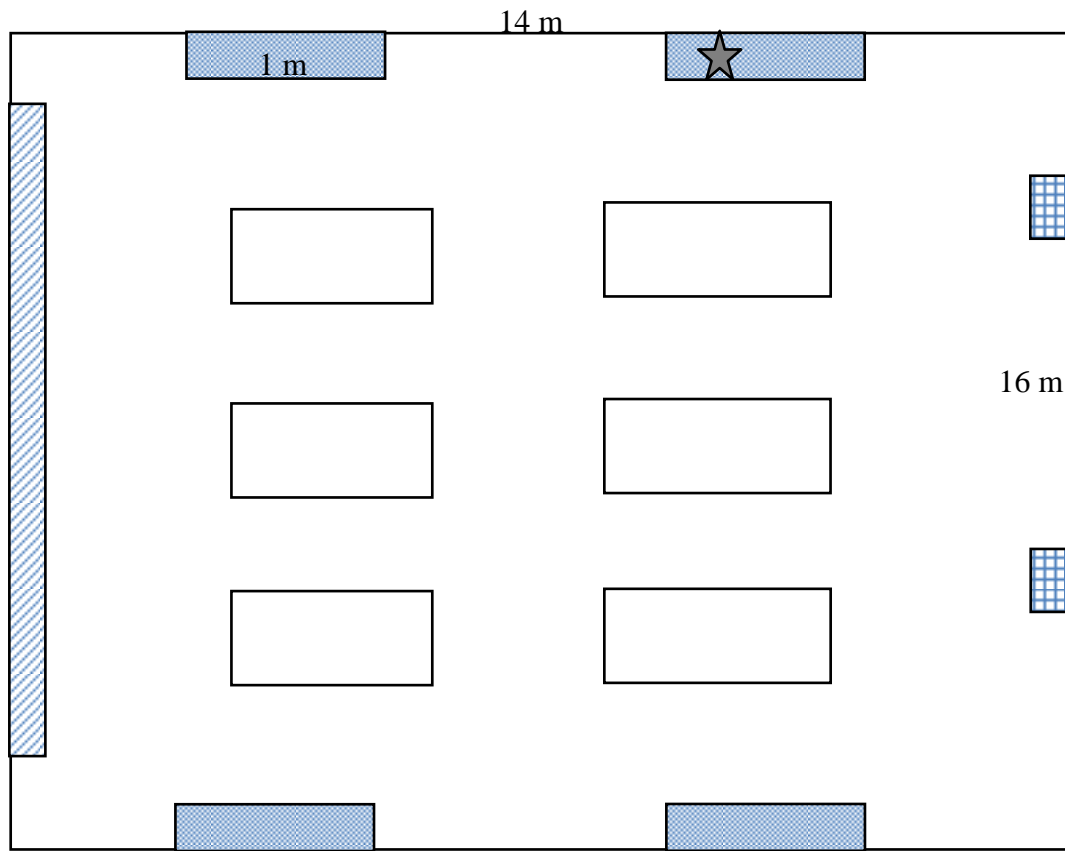







Figure F-6 Diagram of central laboratory, Mahidol University

-  Window
-  Door
-  Bench
-  Hood
-  Ethyl acetate sampling point

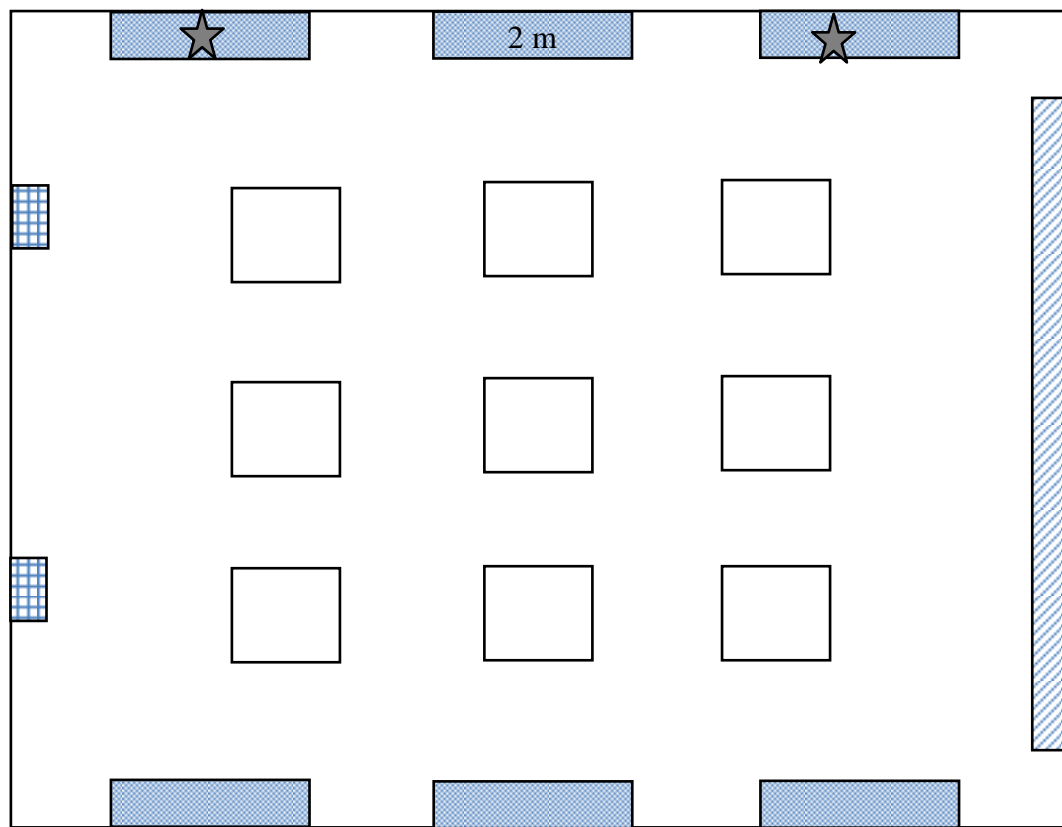







Figure F-7 Diagram of PTT-Global Chemical laboratory

-  Window
-  Door
-  Bench
-  Hood
-  Isopropyl alcohol and toluene sampling point

BIOGRAPHY

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