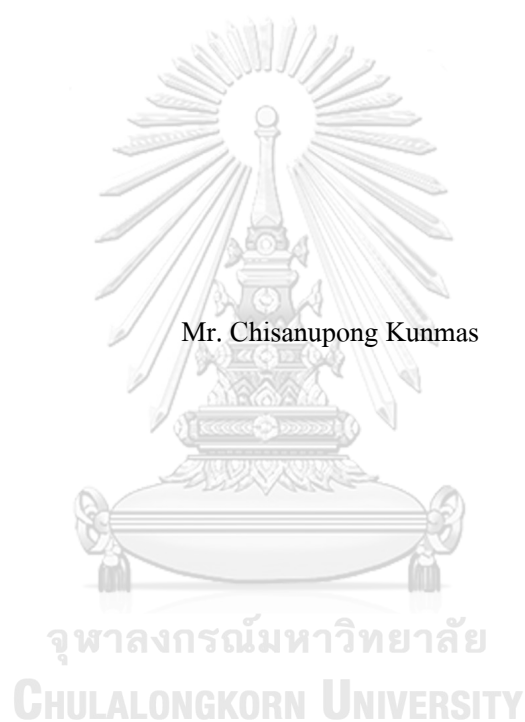DEVELOPMENT OF SPREADSHEET-BASED SIMULATION TO REDUCE NUMBER OF

EXPERIMENTAL TRIALS IN SEPARATION WITH COMPREHENSIVE TWO-

DIMENSIONAL GAS CHROMATOGRAPHY

Mr. Chisanupong Kunmas

จุฬาลงกรณ์มหาวิทยาลัย

CHULALONGKORN UNIVERSITY

A Thesis Submitted in Partial Fulfillment of the Requirements

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การพัฒนาการจำลองบนฐานแผ่นตารางทำการเพื่อลดจำนวนการทดลองในการแยกสารด้วยแก๊ส
โครมาโทกราฟีสองมิติแบบทั่วถึง

นายชิษณุพงศ์ คุณมาศ

Thesis Title	DEVELOPMENT OF SPREADSHEET-BASED SIMULATION TO REDUCE NUMBER OF EXPERIMENTAL TRIALS IN SEPARATION WITH COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY
By	Mr. Chisanupong Kunmas
Field of Study	Green Chemistry and Sustainability
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ชิษณุพงศ์ คุณมาศ : การพัฒนาการจำลองบนฐานแผ่นตารางทำการเพื่อลดจำนวนการทดลองใน
การแยกสารด้วยแก๊สโครมาโทกราฟีสองมิติแบบทั่วถึง. (DEVELOPMENT OF
SPREADSHEET-BASED SIMULATION TO REDUCE NUMBER OF EXPERIMENTAL
TRIALS IN SEPARATION WITH COMPREHENSIVE TWO-DIMENSIONAL GAS
CHROMATOGRAPHY) อ.ที่ปรึกษาหลัก : ผศ. ดร.ชฎิล กุลสิงห์

การพัฒนาวิธีการและการหาสภาวการณ์ทดลองที่ดีที่สุดในแก๊สโครมาโตกราฟีสองมิติแบบ
ทั่วถึง (GC´GC) เป็นกระบวนการที่ต้องมีการใช้การทดลองเป็นจำนวนมากเพื่อให้จำนวนสารที่แยกได้ในแต่
ละตัวอย่างมีจำนวนสูงที่สุด โดยที่นักเรียนในชั้นเรียนแบบบรรยายทั่วไปจะไม่สามารถพัฒนาทักษะเหล่านี้ได้
ในขณะที่พวกเขาสามารถได้ทักษะเหล่านี้ในห้องปฏิบัติการ แต่จะใช้งบประมาณ พลังงานและเวลาเป็นจำนวน
มาก วิทยานิพนธ์นี้จะพัฒนาแผ่นตารางทำการในรูปแบบ Microsoft Excel เพื่อจำลองกราฟเวลาของพีคใน
GC´GC และจำนวนพีคที่สามารถแยกได้ สำหรับตัวอย่างที่กำหนดภายในไม่กี่มิลลิวินาที การประยุกต์ใช้
แนวทางนี้จะลดค่าใช้จ่ายในการทดลอง เพื่อที่จะส่งเสริมทักษะการหาสภาวการทดลองที่ดีที่สุดของนักเรียน
และสามารถทำได้ภายในระยะเวลาไม่กี่ชั่วโมงของชั้นเรียนแบบบรรยาย วิทยานิพนธ์นี้จะแสดงให้เห็นถึงข้อ
ได้เปรียบนี้โดยการแจกแผ่นตารางจำลองการทดลองให้กับนักศึกษา 25 คนในระดับปริญญาตรี ปริญญาโท
และปริญญาเอก จากนั้นพวกเขาได้รับคำแนะนำเกี่ยวกับวิธีการใช้งานแผ่นตารางทำการและการฝึกฝน โดยมี
การกำหนดเป้าหมายการแยกสารที่กำหนดให้ สำหรับตัวโปรแกรมนี้มีตัวแปรการทดลอง GCxGC ที่สามารถ
เปลี่ยนแปลงได้โดยที่จะให้ผลลัพธ์ที่แตกต่างกัน ตัวแปรที่จะเปลี่ยนได้นั้นได้แก่ความยาวคอลัมน์ อัตราการ
ไหลของแก๊ส อุณหภูมิในเตาตั้งต้น อัตราการเพิ่มของอุณหภูมิ คอลัมน์แรก และคอลัมน์ที่สอง หลังจากนั้น
นักเรียนจะทำการทดสอบแยกตัวอย่างสารตัวอย่างเคโรซีนที่ประกอบไปด้วยสารประกอบทั้งหมด 641 สาร
พวกเขาได้คะแนนเฉลี่ย 12 คะแนน จากคะแนนเต็ม 15 คะแนน ซึ่งสอดคล้องกับค่าเฉลี่ยของจำนวนพีคที่แยก
ได้ที่ 226 พีค จากจำนวนสูงสุดในอุดมคติคือ 235 พีค นั่นหมายความว่านักเรียนสามารถแยกได้ถึง 96% ของ
จำนวนพีคในอุดมคติที่ควรจะแยกได้สำหรับตัวอย่างนี้ จากผลนี้สามารถระบุได้ถึงทักษะการลองผิดลองถูกที่
นักเรียนสามารถเรียนรู้ได้ภายในเวลาเรียน 2-3 ชั่วโมง เมื่อเทียบกับการทดลองจริงใน GCxGC ที่นักเรียนแต่ละ
คนต้องใช้เวลาประมาณ 30 ชั่วโมงเพื่อที่จะได้เรียนรู้ทักษะเหล่านี้ นอกจากนี้ผลการจำลองยังสอดคล้องกับผล
การทดลองการแยกตัวอย่างน้ำมันหอมระเหยโดยมีค่าสัมประสิทธิ์สหสัมพันธ์ (R^2) ระหว่างเวลาของพีคจาก
การจำลองและจากการทดลองในช่วง 0.63 ถึง 0.96

สาขาวิชา	เคมีสีเขียวและความยั่งยืน	ลายมือชื่อนิสิต ....
ปีการศึกษา	2566	ลายมือชื่อ อ.ที่ปรึกษาหลัก ....

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KEYWORD: Analytical Chemistry, Computer-Based Learning, Chromatography, Computational Chemistry, Green chemistry

Chisanupong Kunmas : DEVELOPMENT OF SPREADSHEET-BASED SIMULATION TO REDUCE NUMBER OF EXPERIMENTAL TRIALS IN SEPARATION WITH COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY. Advisor: Asst. Prof. CHADIN KULSING, Ph.D.

Method development and optimization in comprehensive two- dimensional gas chromatography (GC′GC) is a process with the requirement to perform a large number of experiments maximizing the number of separated components in each sample. These are the skills which cannot be developed by students in a general lecture class; while, they can be achieved in a laboratory although with consumption of large amount of budget, energy and time. This thesis developed a spreadsheet in Microsoft Excel format to simulate a GC′GC retention time plot and a number of separated peaks for a given sample within a few milliseconds. Application of this approach waives the experimental expense in enhancing the optimization skills of students and can be performed within a short period of time such as in a few hours of a lecture class. The thesis demonstrated this advantage by distributing the spreadsheet simulation to the group of 25 students consisting of bachelor, master and PhD students. They were then instructed on how to use the spreadsheet simulation and practice with a given separation goal. In this program, the GC′GC parameters, which can be changed leading to different results, include column lengths, gas flow rate, initial oven temperature, temperature increase rate, and the first and the second columns. The students then performed the test to separate a model kerosene sample containing 641 compounds. They showed the average score of 12 out of 15 corresponding to the average number of separated peaks of 226. The students could achieve 96% of 235 separated peaks obtained from the ideally optimized condition for this sample. This could also be an indicative of sufficient trial-and error skills that the students could learn within the a few hours learning time compared with ~30 hours of the actual GC′GC experiments that each student needed to spent on learning such skills. In addition, the simulated results were in agreement with the experimental separation of an essential sample with the correlation coefficients (R^2) between the simulated and experimented peak retention times ranging from 0.63 to 0.96.

Field of Study:	Green Chemistry and Sustainability	Student's Signature ....
Academic Year:	2023	Advisor's Signature ....

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LIST OF ABBREVIATUINS

GCxGC   Comprehensive two-dimensional gas chromatography

1D   One dimensional

2D   Two dimensional

DS   Dean switch

ECD   Electron capture detector

FID   Flame ionization detector

FPD   Flame photometric detector

GC   Gas chromatography

HPLC   High performance liquid chromatography

IL   Ionic liquids

MD   Multidimensional

MS   Mass spectrometer

THQ   Tetrahydroquinolin

CHAPTER I

INTRODUCTION

1.1 Problem definition

Comprehensive two-dimension gas chromatography (GC×GC) is one of the most powerful separation methods to separate volatile compounds resulting in molecular-based fingerprint of each complex sample such as pharmaceutical, illicit drugs, petroleum, food, beverage and environmental. GC×GC could involve a process performing a large number of trial-and-error experiments in order to maximize the number of separated components in each sample. Thus, the optimization skills could not be developed by students in a general lecture class. However, they could learn such skills through experiments in a laboratory which can be achieved with consumption of large amount of budget and time where more than 100 experimental trials could be required for each to understand the concept. This also requires expensive resource and maintenance which are generally not suitable for the general teaching. This thesis thus develops and applies the new simulation approach enabling every student to practice the GC×GC optimization in a lecture class.

1.2 Literature review

Comprehensive two-dimensional gas chromatography (GC×GC) is one of the most powerful analytical methods to separate volatile chemical compounds resulting in molecular-based fingerprint of each complex sample such as pharmaceutical, illicit drugs, petroleum, food, beverage and environmental (Marriott et al., 2012). This technique uses two columns with different selectivity as well as a device located between these columns that offers a modulation process between the columns (Nolvachai et al., 2015b). This device is called as modulator. GC×GC performance is greater than one dimensional (1D) GC in terms of higher separation efficiency, resolution and analyte peak capacity as well as an improved detection limit, *e.g.* the result of the cryogenic refocusing effect (Nolvachai et al., 2015a). Conventional stationary phases, such as the materials based on R,R'-polysiloxane, arylene or poly(ethylene glycol),

provide a separation mainly based on polar/non-polar interactions and analyte vapour pressure differences. The polarities of these GC phases are indicated by the number of phenyl, fluorinated alkyl, or other functional groups of each phase. Apart from these, ionic liquids (IL) have been commercialized and applied for a wide range of applications in chemistry mainly because of their characteristic adaptable properties. They have been identified as the innovation "most likely to shape the 21st century" with the potential 'green' application as solvents to dissolve almost any chemicals (Ghandi, 2014). IL have become attractive GC stationary phase materials which provide several advantages such as their high polarity, high viscosity and low vapour pressure arising from their ionic nature, chemical flexibility of their organic part, and thermal stability of their inorganic parts (Anderson et al., 2005). The applications included separation of fatty acid methyl esters, polychlorinated biphenyls, pesticides and sulfur or nitrogen containing compounds in different sample matrices, as compared with other phases (Poole & Lenca, 2014; Zeng et al., 2013).

General optimization process in GC×GC could involve a number of trial-and-error experiments in selection of the two columns and separation condition such as column dimensions, flow rate and temperature program (Nolvachai et al., 2016). In research and educational areas, each student needs to perform hundreds of experiments just to perceive the optimization concepts. This requires the long investigation time, high energy consumption and high operation cost. One dimensional GC has been taught under different topics in high school or Bachelor (such as 2nd year analytical chemistry). However, students still show difficulty in understanding the details and obtaining the critical thinking skills relevant to practical GC challenges (Thaveesangsakulthai & Kulsing, 2021). This is more difficult for understanding concepts of optimization in GC×GC due to the more variable parameters with much higher operation cost, energy consumption and waste generation.

Computer simulation approaches have been applied for decades to support the learning of optimization process in 1D chromatography. This includes free software (Armitage, 1999) or freely available websites such as GC simulator (Abbott, n.d.). This could support learning of key

parameters such as column length and diameter, stationary phase thickness, diffusion coefficient, flow rate and distribution coefficient of model analytes (Abbott, n.d.). The simulation software has also been reported, enabling chromatographic separations in the classroom for undergraduate students or general students. In this case, students were able to investigate various experimental parameters, including high performance liquid chromatography (HPLC) throughput, column size, particle size, and mobile/stationary phase compatibility (Smith & Villaescusa, 2003). In addition, the other research group applied two simulation exercises in a separation science course for upper-division undergraduate students (Stone, 2007) varying different chromatographic parameters on the simulated chromatograms. With the freely available software, either empirical compounds or limited number of separated compounds have been reported. This is often not suitable for practical sample optimization (Inc, n.d.). Alternatively, the commercial software such as Gas Chromatography Simulation & Optimization Software (GC-SOS) (Company, n.d.), ACD/LC and GC Simulator (Company, n.d.) can be applied for a larger set of compounds with the capability to investigate a wider range of experimental conditions such as column variation. The recent work illustrated Microsoft Excel spreadsheet-based simulation platform assisting students to practice optimization of the experiments in GC (Thaveesangsakulthai & Kulsing, 2021). There have been several papers reporting simulation in GC×GC (Kulsing et al., 2016; Pojjanapornpun et al., 2019; Ren et al., 2007; Siriviboon et al., 2019) mainly focusing on optimization of the experimental conditions towards each sample analysis (Kulsing et al., 2020). They also focused on improved understanding of the theoretical concepts (Kulsing et al., 2018; Nolvachai et al., 2019), as well as improved data analysis approaches (Kakanopas et al., 2022; Prodhan et al., 2018; Veenaas et al., 2018). Unfortunately, the spreadsheet simulation approach to support learning in two-dimensional GC has not been reported.

1.3 Objective

To develop approach for simulation of GC×GC results using Microsoft Excel spreadsheets and to apply this approach allowing students to perform column selection and experimental design in GC×GC. The spreadsheet is applicable for simulation of retention time plots in GC×GC under different experimental condition as well as the number of separated peaks under different experimental condition.

CHAPTER II

THEORY

2.1 Gas Chromatography (GC)

GC is an analytical technique used to separate the chemical components of a sample mixture before detection to determine their presence or absence as well as to quantify their contents in the sample (Marriott, 2005). The word chromatography comes from the Greek root words chroma and graph and translates to "color writing." GC is a technique that separates a mixture of chemicals by letting them move slowly past another substance, typically a liquid or solid. In essence, we have a gas moving over the surface of something else in another state of matter (a liquid or solid) that stays where it is. The moving substance is called the mobile phase and the substance modified inside a column is the stationary phase. GC uses an inert or unreactive carrier gas as the mobile phase, and the stationary phase is generally a thin layer of liquid or polymer. As the mobile phase moves, a sample is separated into its individual components along the stationary phase prior to their detection.

2.1.1 Carrier gas

Carrier gas is an inert gas and mobile phase. It is not reacting with the stationary phase or the sample component. The example of carrier gas are nitrogen, argon and helium. It can be purified to remove traces of oxygen, water and hydrocarbons. The choice of carrier gas is often based on the type of the detector that applied to which is selected to result in good detector response for analytes, as well as inexpensive and easily available and most importance, it is safe to use.

2.1.2 Injector

An injector is a chamber that the sample is transferred into the instrument. The injector will heat the sample to be vapor that will be taken into the column by carrier gas. The

choice of injection system depends on the column type and sample component. The most commonly used type with capillary column is the heated split/splitless injector that can operate in split and splitless modes. The selection of injection mode depends on compound concentrations in samples.

Both split and splitless injection mode are performed under high injection temperature that make the samples and solvent to vaporize. Throughout the GC run, the injection temperature is constant. The split injection is used for neat samples with relatively high concentration while the splitless mode is applied when samples contain analytes at trace levels. Under the split mode, the sample is injected and it vaporizes into carrier gas stream. Only the small portion of the sample and solvent is transferred into GC column and the rest will be vented to waste. The amount of analyte entering the column can be calculated according to **Equation 1** as

$$\text{Split ratio} = \frac{\text{Column flow+Vent flow}}{\text{Column flow}} \tag{1}$$

In splitless mode, the sample is introduced into the heated linear as in split injection and it is brought into the gas phase without sample discrimination during injection. This introduces all the injected amount of the sample and solvent onto GC column inlet. This technique is useful for trace analysis of the compound in the sample or the compound with narrow boiling-point range, but this is not suitable for injection of thermally labile compounds.

2.1.3 Column

A column is connected with the injector and detector inside a GC oven. The column dimension varies in length and internal diameter depending on the application type. There are two general column types, packed and capillary. Sample components are separated into column with the separation result depending on interaction between stationary phase and mobile phase and

mainly governed by the chemistry of stationary phase materials. Conventional stationary phases include R,R'-polysiloxane, arylene or poly(ethylene glycol). They provide a separation based on polar/non-polar interactions and analyte vapor pressure differences. Their polarities could be adjusted with the number of phenyl, fluorinated alkyl, or other functional groups. IL stationary phase have also been applied for a wide range of applications such as separations of fatty acid methyl esters, polychlorinated biphenyls, pesticides and sulfur or nitrogen containing compounds in different sample matrices (Kulsing et al., 2015).

2.1.4 Detector

The physicochemical property of the analyte responds to the detector. Most of the detectors are sensitive and generate electronic signals for the data system to further produce a chromatogram. The common detectors used in GC include the flame ionization detector (FID), flame photometric detector (FPD), the electron capture detector (ECD) and mass spectrometer (MS) (Klee, 2012).

2.1.5 Mass spectrometry (MS)

Mass spectrometry is an analytical technique that is suitable and powerful tool for compound analysis to positively identify compounds and quantity known compounds within a sample. Hyphenation with GC allows separation of compounds prior to the MS detection (Klee, 2012). A typical result is shown as a MS spectrum of each separated compound which is a plot of ion intensity (counts) vs mass to charge ratio.

2.2 Multidimensional (MD) Chromatography

Multidimensional chromatography is a separation technique which is an important analytical tool because it provides high chromatographic resolution for separating complex mixtures and difficult to separate substances such as petrochemistry, metabolomics, environmental, and flavor and fragrance science (Marriott, 2005; Seeley & Seeley, 2013).

MD chromatography is a powerful separation technique that has been developed in the past few years. This method is appropriate with the analysis of highly complex samples. Different separation mechanism is exploited in each dimension for improving the resolution in the separation. The separation performance is based on the sample properties and involves multiple chromatographic steps. MD chromatography offers superior peak capacity and has the potential to overcome the limitations of one-dimensional chromatography. MD chromatography originated from simple techniques where only target fractions from the first dimensional separation are isolated and transferred to undergo second dimensional separation. The separation performance depends on several parameters such as sample types, stationary phase types, first and second column lengths, flow rates, temperature programs (Nolvachai et al., 2018).

2.3 Comprehensive two-dimensional gas chromatography (GC✕GC)

GC×GC is a class of MDGC comprehensively separating all the sample components using two chromatographic columns with different selectivity. Having two dimensions of separation means that GC×GC provides greater separation capacity than the one-dimensional GC, enabling complex mixtures to be resolved (Marriott, 2018). GC×GC generally employs two columns: a long primary column (typically 20–30 m) and a short secondary column (1–5 m), **Figure 1**. The two columns are sequentially connected with a modulator. As in one-dimensional GC, the sample is introduced into a heated port and swept through the primary column by a carrier gas. The peaks that elute are then sampled (ideally three or four times per peak) and each fraction is re-injected as a narrow chromatographic band into the secondary column. Passage through the secondary column is quick to ensure sharp peaks and no band overlap, with elution usually taking place in under 10 seconds. Following elution from the second column, detection takes place, and the signal is processed to generate a three-dimensional 'surface plot' (which can alternatively be viewed as a two-dimensional 'contour plot').
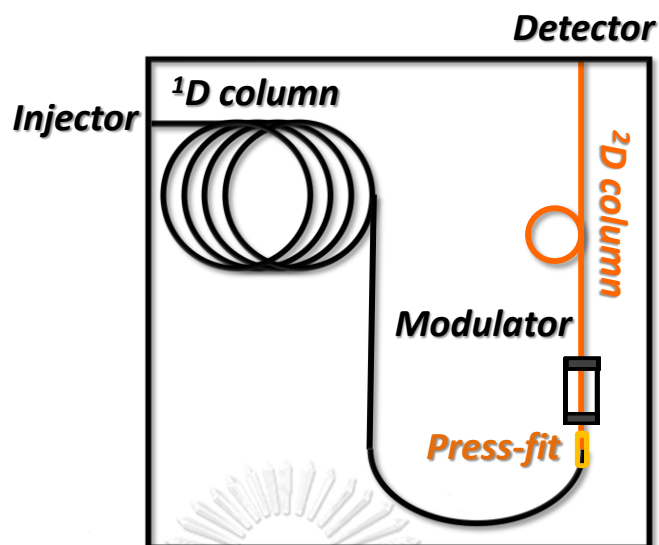
Figure 1. The Gas Chromatography diagram.

2.4 Optimization process

Optimization process is a systematic approach which aims to find the optimal solution for a particular function under constraints. The solution or alternative could involve the most cost-effective and achieve the best result. Optimization in business usually involves aiming for the highest profits and lowest costs. In other words, it is the act or process of making something as perfect, fully functional, or effective as possible. In computer science and mathematics, this is the selection of the best element (with regard to some criteria) from given sets of available alternatives. More generally, optimization includes finding best available values of some objective function given a defined set of constraints, including a variety of different types of options.

2.5 Simulation-based learning

Simulation-based learning is training in a virtual environment that mimics real-world activities and scenarios. Trainees can apply practical information and skills not merely by reading

theory books or listening to lectures but also by engaging in physical, hands-on activities. The term "simulation" refers to mimicking a real-life process to deliver a realistic experience in a controlled setting. It is a place where you can learn from your mistakes without causing any harm. Such learning allows students to try out various scenarios and learn what works and what doesn't; to understand how they arrived at correct and incorrect responses. This method of trial-and-error provides learners with the information and confidence they need to put their new talents to use in the real world.

The effectiveness of simulation-based learning is high because it considers learners' preferred learning styles. Simulation-based training is a very successful and cost-effective method of imparting vital skills to students. Educational simulation is a teaching strategy that puts students in situations where they must actively solve challenges to assess their knowledge and skills. The teacher sets the restrictions to ensure a safe atmosphere for hands-on learning. Students must immediately assess the issue, choose the best course of action, and follow necessary procedural steps when engaging in a scenario. Educators can then evaluate whether students have grasped the subject and whether they are applying their knowledge.

Learning in a controlled and safe setting gives students valuable hands-on experience that combines fundamental theoretical concepts with interactive, computer-simulated scenarios. Given below are a few advantages of simulation-based learning:

1) Simulators can help individuals improve their skills and learn from their failures.

2) Trainees can better understand the implications of their actions and how important it is to prevent them from happening again.

3) Users can receive fast feedback, enabling them to understand what exactly went wrong or right. They also know what is causing the problem and how to fix it.

4) Individuals and groups of learners put their learnings into practice by applying their critical thinking skills. Some examples of simulation-based learning include

knowledge-in-action procedures, decision-making, and effective communication. Simulation, in essence, allows for the investigation of human elements and their interactions with their surroundings.

5) Simulator-based learning can be set up at specific times, places, and circumstances and then replayed as needed. It can be done with minimal setup in businesses and homes, or it can be done in incredible high-tech simulation centres.

6) Simulation-based learning can be tailored to meet the needs of beginners, intermediates, and experts and adapted to the changing abilities of learners.

7) Simulators deepen the learning conversation, boost motivation, and help novices become experts by providing insights from another participant's point of view.

8) This learning technique includes various debriefing options, such as video feedback and peer evaluation.

CHAPTER III

EXPERIMENTALS

3.1 Development of spreadsheet

Develop the spreadsheet for simulation of GC×GC results of the kerosene model using different experimental conditions. This starts from the concept of linear solvation energy relationship (LSER) which is the concept describing that analyte retention (stationary phase/compound interaction) can be deconvoluted into different interaction types between each analyte and the stationary phase. It is hypothesised that each interaction type can be experimentally scaled by the product of analyte and stationary phase descriptors with the general relationship under a constant temperature separation (Kulsing et al., 2014) as

$$\log k = c + eE + sS + aA + bB + lL \tag{2}$$

where $e{\times}E$ involves dispersity-related interaction, $s{\times}S$ involves dipole-type interaction, $b{\times}B$ involves H-bonding with basic analyte, $a{\times}A$ involves H-bonding with acid analyte, and $l{\times}L$ involves cavity formation/dispersion.

The related equations to predict the retention time in the first and second dimensional separations ($^{1}t_{R}$ and $^{2}t_{R}$) can then be introduced. For a constant flow separation, t_{R} of a compound in either first or second dimension on a given set of GC columns and dimensions, flow rate and temperature program (starting temperature, T_{start}, and temperature increase rate, γ) according to (Siriviboon et al., 2019)

$$t_{R} = \frac{T - T_{stat}}{\gamma} \tag{3}$$

where

$$T = -\frac{1}{b}\ln\left(e^{-\gamma^{t}m^{b}}\left(e^{-bT_{0}} + A\right) - A\right) \tag{4}.$$

t_M is void time of the column in separation and can be approximated for a given set of column dimensions and phases. A and b are constants depending on the separated compound and stationary phase on each dimensional separation.

$$A = 10(C_{e_i} E_j + C_{s_i} S_j + C_{a_i} A_j + C_{b_i} B_j + C_{l_i} L_j + C_{c_i}) \tag{5}$$

$$b = (\log_e 10)(M_{e_i} E_j + M_{s_i} S_j + M_{a_i} A_j + M_{b_i} B_j + M_{l_i} L_j + M_{c_i}) \tag{6}$$

With a conventional PC (Intel® Core™ i5-3320M CPU @ 2.6GHz, 8 GB RAM), the simulation can be obtained within a second. The apparent number of separated peaks (P_{app}) was then simulated in each GC experiment according to the previously established concept (Thaveesangsakulthai & Kulsing, 2021). P_{app} is estimated from the total number of peaks with baseline separation in a GC result. Average peak width at baseline (w_b) at different experimental condition which can be approximated according to the theoretical plate height (H) concept according to the equation

$$W_{b,I} = 4\sqrt{\frac{H_i(t_{R,i})^2}{L_i}} \tag{7}$$

According to the experimental data, H will be approximated in this thesis to be 0.001 m. The related Microsoft Excel spreadsheet allowing simulation of GC×GC results for a given set of input parameters will then be constructed.

Calculation of the parameters (**Equation 4**) were performed using several excel formula. For example, analyte elution temperature on the first and second columns (T1 and T2) can be set according to the following formula.

T1 =-1/'database for constant values'!I3*LN(EXP(-Calculation!$B$10*Calculation!$B$15* 'database for constant values'!I3)*('database for constant values'!H3+EXP(-'database for constant values'!I3*Calculation!$B$9))-'database for constant values'!H3)   (8), and

T2 = -1/'database for constant values'!K3*LN(EXP(-Calculation!$B$10*Calculation!$C$15 *'database for constant values'!K3)*('database for constant values'!J3+EXP(-'database for constant values'!K3*'Inner Calculation'!A2))-'database for constant values'!J3)   (9)

Calculation of ^1t_R and ^2t_R can then be set according to the following formula.

$$^1t_R = (A2\text{-Calculation!}\$B\$9)/\text{Calculation!}\$B\$10 \qquad (10)$$

$$^2t_R = (B2\text{-A2})/\text{Calculation!}\$B\$10*60 \qquad (11)$$

The data of the constant values applied in this thesis are listed for the stationary phase and the analytes in **Table 1** and **Table 2**, respectively. These are used for calculation of retention time.

Table 1. Constant values for the applied stationary phase with the slope (M) and intercept (C) showing linear dependency of each stationary phase descriptor on the applied temperature, obtained from the reference (Siriviboon et al., 2019).

Stationary phase		Stationary phase descriptor					
		e	*s*	*a*	*b*	*l*	*c*
IL59	M	-0.001	-0.003	-0.007	-0.002	-0.002	0.000
	C	0.140	1.809	2.175	0.568	0.655	-2.919
IL82	M	-0.001	-0.003	-0.008	-0.004	-0.003	0.000
	C	0.307	1.988	2.281	0.929	0.661	-3.050
[P66614][FeCl$_4$]	M	0.001	-0.003	-0.008	-0.003	-0.003	-0.003
	C	-0.327	1.683	1.930	0.247	0.937	-2.923

DB-1	M	0.001	-0.001	-0.003	0.000	-0.003	-0.002
	C	-0.129	0.305	0.520	0.000	0.864	-1.816
Rxi17	M	0.001	-0.003	-0.002	0.000	-0.002	0.000
	C	0.011	1.141	0.618	0.057	0.832	-2.585
HP-5	M	0.001	-0.001	-0.002	0.000	-0.002	-0.001
	C	-0.126	0.452	0.398	0.000	0.771	-2.197
HP-88	M	0.000	-0.004	-0.005	0.000	-0.001	-0.001
	C	0.108	1.871	2.101	0.000	0.487	-2.756
HP-INNOWAX	M	0.001	-0.005	-0.011	0.000	-0.002	-0.001
	C	0.109	2.001	3.231	0.000	0.693	-2.557
IL76	M	-0.002	-0.002	-0.011	-0.001	-0.003	0.000
	C	0.348	1.800	2.857	0.468	0.676	-3.128
IL100	M	-0.001	-0.008	-0.013	-0.006	-0.003	-0.001
	C	0.262	2.656	2.934	1.247	0.670	-2.986
$[C4mim][FeCl_4]$	M	-0.001	-0.004	0.002	-0.001	-0.002	-0.006
	C	0.313	2.157	1.770	0.863	0.703	-2.703
Rtx-440	M	0.001	-0.001	-0.001	0.000	-0.002	0.000
	C	-0.066	0.507	0.337	0.000	0.696	-2.343
Rxi-50	M	0.000	-0.002	-0.001	-0.001	-0.002	0.000
	C	0.098	0.835	0.411	0.245	0.636	-2.107
Rtx-OPP	M	0.001	-0.002	-0.001	0.000	-0.002	0.000

Rtx-OPP	C	-0.293	0.993	0.240	0.000	0.613	-2.513
DB-1701	M	0.001	-0.002	-0.003	0.000	-0.002	0.000
	C	-0.163	0.841	0.995	0.000	0.675	-2.109
DB-225	M	0.001	-0.003	-0.004	0.000	-0.002	0.000
	C	-0.066	1.460	1.448	0.000	0.587	-2.839

Table 2. Constant values for the applied 641 compounds obtained from the reference (Siriviboon et al., 2019).

Compound name	Constants				
	E	S	A	B	L
(3-Methyl-5-hexen-1-yn-1-yl)benzene	0.1	0.12	0.06	0.02	0.09
5-(4-Pentyn-1-yl)indane	0.1	0.12	0.06	0.02	0.09
(1-Cyclohexen-1-ylethynyl)benzene	0.1	0.12	0.06	0.02	0.09
(Cyclohexylethynyl)benzene	0.1	0.12	0.06	0.02	0.09
(1Z)-1-Octen-3-yn-1-ylbenzene	0.1	0.12	0.06	0.02	0.09
(1E)-1-Octen-3-yn-1-ylbenzene	0.1	0.12	0.06	0.02	0.09
2-Ethynyl-4-methyl-1-[(2S)-4-penten-2-yl]benzene	0.1	0.12	0.06	0.02	0.09
1-(1-Hexyn-1-yl)-2-vinylbenzene	0.1	0.12	0.06	0.02	0.09
[3-(1-Cyclohexen-1-yl)-2-propyn-1-yl]benzene	0.1	0.12	0.06	0.02	0.09
1,3,5-Trimethyl-2-[(1E)-1-penten-3-yn-1-yl]benzene	0.17	0.13	0.01	0.01	0.72
(5-Methyl-3,4-octadien-6-yn-1-yl)benzene	0.17	0.13	0.01	0.01	0.72
methanal	0.22	0.62	0	0.33	0.73
ethanal	0.21	0.67	0	0.45	1.23
1-Octen-5-yn-4-ylbenzene	0.16	0.1	0.01	0.1	1.26
dimethylether	0.19	0.36	0.01	0.44	1.39
2-propanone	0.18	0.7	0.4	0.49	1.7
acetone (=propanone)	0.28	0.7	0.03	0.49	1.79

propanal	0.2	0.65	0	0.45	1.82
furan	0.54	0.64	0.02	0.19	2.18
cyclopropanpone	0.39	0.79	0.04	0.47	2.2
butanal	0.19	0.65	0	0.45	2.27
1,4-Nonadiyn-1-ylbenzene	0.14	0.1	0	0.1	2.28
2-butanone	0.17	0.7	0	0.51	2.29
methyl propanone	0.27	0.71	0	0.52	2.34
methoxymethylamine	0.38	0.72	0.33	0.69	2.49
cyclobutenone	0.44	0.87	0.02	0.47	2.54
cyclobutanone	0.39	0.81	0.02	0.52	2.61
2-pentanone	0.14	0.68	0	0.51	2.76
heptyne	0.13	0.1	0	0.1	2.76
Pentanal	0.16	0.65	0	0.45	2.77
ethyl propanone	0.26	0.69	0	0.53	2.82
ethyl ketone = ethyl ethanone	0.27	0.68	0	0.54	2.86
isoheptene	0.18	0.19	0	0.17	3.09
isooctene	0.18	0.19	0	0.17	3.09
furanone	0.55	1.02	0.02	0.51	3.1
pentanol	0.32	0.47	0.37	0.51	3.11
iso-heptane	0.12	0.09	0	0.1	3.11
methyl isobutyl ketone	0.23	0.67	0	0.54	3.13
1,6-heptadiene	0.26	0.26	0	0.18	3.15
1,3-heptadiene	0.3	0.31	0	0.17	3.17
1,4-heptadiene	0.26	0.22	0	0.17	3.17
heptene	0.19	0.2	0	0.16	3.17
1,5-heptadiene	0.29	0.22	0	0.18	3.17
[(3E)-3-Ethyl-3-hexen-1-yn-1-yl]benzene	0.26	0.19	0	0.18	3.2
cyclopentenone	0.51	0.89	0.02	0.52	3.2
cyclopentadienone	0.68	0.9	0.03	0.48	3.21

cyclopentanone	0.44	0.85	0.01	0.55	3.22
n-heptane	0.14	0.1	0	0.1	3.25
octyne	0.14	0.1	0	0.1	3.25
dimethyl furan	0.65	0.77	0.01	0.31	3.26
2-Hexanone	0.14	0.68	0	0.51	3.29
ethyl butanone	0.25	0.68	0	0.54	3.32
methyl pentanone	0.25	0.69	0	0.54	3.33
2-Hexanol	0.19	0.36	0.33	0.56	3.34
Hexanal	0.15	0.65	0	0.45	3.37
2,2,4-Trimethylpentane	0.14	0.1	0	0.12	3.38
2,2,4-Trimethylpentene	0.14	0.1	0	0.12	3.38
methylbenzene	0.71	0.6	0	0.22	3.42
methyl cyclohexane	0.31	0.17	0	0.1	3.47
ethyl cyclopentene	0.39	0.23	0	0.18	3.57
diisopropyl ketone	0.23	0.63	0	0.55	3.6
1-Hexanol	0.21	0.42	0.37	0.48	3.61
1,2,4-Trimethylpentane	0.14	0.08	0	0.1	3.64
1,2,4-Trimethylpentene	0.27	0.19	0	0.19	3.65
iso-octane	0.13	0.09	0	0.1	3.66
cyclohexadienone	0.7	0.9	0.01	0.53	3.66
octene	0.19	0.2	0	0.17	3.67
cyclohexenone	0.52	0.89	0	0.55	3.68
1,5-octadiene	0.27	0.22	0	0.17	3.7
1,6-octadiene	0.27	0.21	0	0.17	3.7
1,4-octadiene	0.26	0.24	0	0.17	3.71
cycloheptene	0.43	0.26	0	0.18	3.71
1,2,3-Trimethylpentane	0.15	0.09	0	0.1	3.71
1,2,3-Trimethylpentene	0.26	0.18	0	0.19	3.72
1,7-octadiene	0.26	0.26	0	0.17	3.72

1,3-octadiene	0.3	0.35	0	0.17	3.73
1-methyl 4-methyl cyclohexane	0.22	0.2	0	0.09	3.73
cyclohexanone	0.46	0.82	0	0.57	3.73
cycloheptane	0.41	0.17	0	0.1	3.75
propyl ketone = propyl propanone	0.24	0.68	0	0.54	3.76
2-Heptanone	0.12	0.68	0	0.51	3.76
cycloheptatrienone	0.5	0.75	0.01	0.46	3.77
n-octane	0.14	0.1	0	0.1	3.78
nonyne	0.14	0.1	0	0.1	3.78
ethyl pentanone	0.24	0.69	0	0.54	3.78
1-methyl 3-methyl cyclohexane	0.24	0.2	0	0.09	3.8
N-isopropyl-2-methoxyethylamine	0.3	0.65	0.15	0.88	3.81
1-methyl 2-methyl cyclohexane	0.26	0.2	0	0.08	3.81
2-heptanone	0.24	0.71	0	0.54	3.81
1-methyl 1-methyl cyclohexane	0.3	0.21	0	0.1	3.86
Heptanal	0.14	0.65	0	0.45	3.86
dimethyl furanone	0.63	0.96	0.02	0.59	3.87
p-Xylene	0.69	0.57	0	0.23	3.89
m-Xylene	0.7	0.57	0	0.23	3.9
propyl cyclopentene	0.37	0.22	0	0.19	3.91
propyl furan	0.64	0.77	0	0.32	3.91
Ethylbenzene	0.72	0.59	0	0.24	3.93
ethyl cyclohexane	0.32	0.16	0	0.11	3.93
o-Xylene	0.72	0.59	0	0.23	3.96
dimethylbenzene	0.72	0.59	0	0.23	3.96
butyl butyl ether	0.17	0.33	0	0.48	4.01
methyl cycloheptane	0.3	0.16	0	0.11	4.02
vinylbenzene	0.88	0.7	0	0.25	4.03
styrene	0.88	0.7	0	0.25	4.03

2,2,4-Trimethylhexane	0.16	0.09	0	0.11	4.06
isopropoxypropylamine	0.33	0.69	0.19	0.83	4.1
2-Heptanol	0.19	0.36	0.33	0.56	4.12
1-Heptanol	0.21	0.42	0.37	0.48	4.12
iso-nonane	0.13	0.09	0	0.11	4.13
1,5-nonadiene	0.27	0.21	0	0.18	4.17
cyclooctene	0.47	0.26	0	0.18	4.17
1,2,3-Trimethylhexane	0.15	0.09	0	0.12	4.17
1,6-nonadiene	0.27	0.21	0	0.18	4.17
1,2,3-Trimethylhexene	0.27	0.16	0	0.19	4.18
1,4-nonadiene	0.26	0.21	0	0.18	4.19
1,2,4-Trimethylhexane	0.15	0.09	0	0.11	4.19
1,3-nonadiene	0.3	0.31	0	0.18	4.19
1,2,4-Trimethylhexene	0.27	0.19	0	0.2	4.2
cycloheptenone	0.49	0.81	0	0.55	4.2
cycloheptanone	0.44	0.74	0	0.56	4.22
nonene	0.2	0.2	0	0.17	4.22
cycloheptadienone	0.64	0.83	0	0.54	4.23
cyclooctane	0.45	0.17	0	0.11	4.24
N-sec-butyl-2-methoxyethylamine	0.29	0.65	0.14	0.87	4.24
n-nonane	0.15	0.1	0	0.11	4.24
decyne	0.15	0.1	0	0.11	4.24
2-Octanone	0.11	0.68	0	0.51	4.26
propyl pentanone	0.25	0.69	0	0.54	4.31
ethyl hexanone	0.25	0.69	0	0.54	4.31
isoPropylbenzene	0.73	0.59	0	0.24	4.32
1,1,2-trimethyl cyclohexane	0.41	0.24	0	0.12	4.33
Octanal	0.14	0.65	0	0.45	4.36
1-ethyl 4-methyl cyclohexane	0.3	0.21	0	0.12	4.37

isopropyl cyclohexane	0.34	0.17	0	0.14	4.38
isopropyl cycloheptane	0.34	0.17	0	0.14	4.38
propylbenzene	0.72	0.62	0	0.25	4.39
1-ethyl 1-methyl cyclohexane	0.38	0.2	0	0.13	4.41
1-methyl 4-ethyl benzene	0.73	0.57	0	0.25	4.41
1-ethyl 3-methyl cyclohexane	0.3	0.22	0	0.13	4.41
1-methyl 3-ethyl benzene	0.73	0.57	0	0.25	4.41
1,2,4-trimethyl cyclohexane	0.35	0.28	0	0.14	4.41
dimethyl cycloheptane	0.33	0.16	0	0.14	4.41
propyl cyclohexane	0.35	0.19	0	0.14	4.42
butyl cyclopentene	0.39	0.22	0	0.21	4.42
1,2,3-trimethyl cyclohexane	0.42	0.28	0	0.14	4.43
1-ethyl 2-methyl cyclohexane	0.33	0.2	0	0.12	4.43
propyl cyclohexene	0.4	0.22	0	0.22	4.43
1-methyl 2-ethyl benzene	0.75	0.59	0	0.25	4.44
1,3,5-trimethyl cyclohexane	0.33	0.28	0	0.13	4.46
ethyl cycloheptane	0.34	0.17	0	0.13	4.46
1,2,4-Trimethylbenzene	0.74	0.59	0	0.26	4.47
ethyl cycloheptene	0.41	0.23	0	0.21	4.47
2,2,4-Trimethylheptane	0.17	0.1	0	0.13	4.52
1,2,3-Trimethylbenzene	0.76	0.61	0	0.26	4.53
butyl furan	0.64	0.8	0	0.35	4.54
diisobutyl ketone	0.23	0.64	0	0.55	4.55
methyl cyclooctane	0.38	0.18	0	0.13	4.6
acetophenone	0.88	0.99	0	0.52	4.61
2-Octanol	0.16	0.36	0.33	0.56	4.62
1-octanol	0.2	0.42	0.37	0.48	4.62
methyl cyclooctene	0.44	0.25	0	0.21	4.64
2-methylanisole (=methoxytoluene)	0.83	0.8	0	0.34	4.65

cyclopentylpropanone	0.42	0.76	0	0.59	4.66
1,5-decadiene	0.28	0.21	0	0.18	4.68
1,6-decadiene	0.28	0.21	0	0.19	4.68
1,3-decadiene	0.31	0.36	0	0.18	4.68
1,4-decadiene	0.27	0.22	0	0.19	4.69
indan	0.89	0.65	0	0.22	4.69
decene	0.21	0.22	0	0.17	4.71
2,4-dimethyl-3-heptanone	0.27	0.67	0	0.57	4.71
iso-decane	0.15	0.1	0	0.12	4.73
1,2,3-Trimethylheptane	0.18	0.1	0	0.13	4.73
2-Nonanone	0.11	0.68	0	0.51	4.74
1,2,3-Trimethylheptene	0.23	0.2	0	0.22	4.76
indene	1.03	0.82	0.01	0.24	4.78
isopentyl cyclopentene	0.39	0.22	0	0.21	4.8
1,2,4-Trimethylheptane	0.17	0.1	0	0.13	4.8
n-decane	0.15	0.11	0	0.11	4.81
undecyne	0.15	0.11	0	0.11	4.81
1,2-dimethyl 4-ethyl benzene	0.74	0.59	0	0.26	4.81
1-methyl 4-propyl cyclohexane	0.32	0.25	0	0.11	4.81
butyl ketone = butyl butanone	0.24	0.7	0	0.53	4.83
cyclononene	0.5	0.26	0	0.2	4.83
1,4-diethylbenzene	0.72	0.55	0	0.25	4.83
butyl pentanone	0.25	0.7	0	0.53	4.84
Nonanal	0.15	0.65	0	0.45	4.86
1,2-dimethyl 3-ethyl benzene	0.75	0.59	0	0.26	4.86
cyclononane	0.49	0.19	0	0.11	4.87
1-methyl 1-propyl cyclohexane	0.41	0.22	0	0.13	4.88
1-methyl 2-propyl benzene	0.74	0.59	0	0.25	4.89
butyl cyclohexane	0.39	0.21	0	0.12	4.89

butylbenzene	0.74	0.64	0	0.25	4.89
1-methyl 2-propyl cyclohexane	0.37	0.26	0	0.11	4.89
1-methyl 3-propyl cyclohexane	0.33	0.24	0	0.11	4.89
1,2,4,5-Tetramethylbenzene	0.75	0.6	0	0.26	4.89
isobutylcyclohexane	0.35	0.21	0	0.13	4.9
1,2,3,4-Tetramethylbenzene	0.77	0.6	0	0.26	4.9
1,3-diethylbenzene	0.72	0.55	0	0.24	4.9
cyclooctanone	0.5	0.75	0	0.57	4.91
1-Methyl-2-[(1E)-5-methyl-1-hexen-3-yn-1-yl]benzene	0.88	0.73	0	0.25	4.91
butyl cyclohexene	0.46	0.24	0	0.21	4.92
cyclooctatrienone	0.73	0.88	0.01	0.53	4.95
2,2,4-Trimethyloctane	0.18	0.11	0	0.14	4.97
1,2-diethylbenzene	0.74	0.57	0	0.25	4.98
propyl cycloheptene	0.43	0.24	0	0.21	4.98
benzyl methyl ketone	0.84	0.94	0	0.64	4.98
divinylbenzene	0.94	0.83	0	0.26	5
Methyl acetophenone (=p-Acetyltoluene)	0.9	1	0	0.53	5.12
2-Nonanol	0.17	0.36	0.33	0.56	5.12
1-Nonanol	0.19	0.42	0.37	0.48	5.12
o-acetyltoluene	0.88	0.99	0	0.53	5.12
Decalin	0.54	0.28	0	0.06	5.16
ethyl anisole	0.86	0.87	0	0.39	5.16
ethyl cyclooctane	0.37	0.18	0	0.12	5.16
m-acetyltoluene	0.89	1	0	0.53	5.17
ethyl cyclooctene	0.47	0.22	0	0.19	5.17
cyclopentyl-2-butanone	0.42	0.81	0	0.58	5.18
1,6-undecadiene	0.27	0.22	0	0.19	5.18
1,5-undecadiene	0.26	0.26	0	0.2	5.18

1,4-undecadiene	0.26	0.26	0	0.2	5.19
1,3-undecadiene	0.3	0.39	0	0.2	5.19
iso-undecane	0.16	0.1	0	0.12	5.2
undecene	0.21	0.23	0	0.17	5.21
Naphthalene	1.23	0.89	0	0.26	5.21
Tetralin	0.92	0.67	0	0.24	5.21
methyl indan	0.97	0.73	0.02	0.24	5.22
2,2,4-Trimethyloctene	0.25	0.21	0	0.22	5.23
2-Decanone	0.11	0.68	0	0.51	5.25
1,2,3-trimethyl 5-ethyl benzene	0.78	0.62	0	0.27	5.28
n-undecane	0.15	0.11	0	0.11	5.3
dodecyne	0.15	0.11	0	0.11	5.3
methyl indene	1.09	0.91	0.03	0.25	5.33
1,2,3-trimethyl 4-ethyl benzene	0.79	0.63	0	0.27	5.35
methyl cyclononane	0.41	0.19	0	0.12	5.36
methyl cyclononene	0.46	0.27	0	0.21	5.36
1-Ethynyl-2-(3-methyl-2-buten-1-yl)benzene	0.8	0.62	0	0.26	5.39
cyclodecane	0.51	0.19	0	0.1	5.41
1-methyl 2-butyl benzene	0.74	0.63	0	0.26	5.42
1,2-Dimethyl-3-propylbenzene	0.75	0.63	0	0.27	5.42
1-methyl 2-butyl cyclohexane	0.42	0.29	0	0.1	5.43
cyclodecene	0.51	0.27	0	0.19	5.43
pentylbenzene	0.74	0.66	0	0.26	5.44
isopentyl cyclohexane	0.37	0.25	0	0.13	5.44
pentyl cyclohexene	0.45	0.28	0	0.21	5.44
1,2-Dimethyl-4-propylbenzene	0.75	0.63	0	0.27	5.46
1-ethyl 4-propyl cyclohexane	0.37	0.29	0	0.11	5.46
Pentamethylbenzene	0.86	0.66	0	0.28	5.47
1-ethyl 2-propyl benzene	0.74	0.62	0	0.25	5.47

methylbutyl cyclohexane	0.42	0.29	0	0.12	5.47
isopropyl ethyl benzene	0.75	0.6	0	0.26	5.49
1,2,3,4-Tetrahydroquinoline (THQ)	1.06	0.94	0.22	0.55	5.51
hexyl cyclopentene	0.44	0.27	0	0.2	5.53
pentyl cyclohexane	0.42	0.25	0	0.12	5.54
benzyl ethyl ketone	0.84	1.01	0	0.57	5.56
p-ethyl acetophenone	0.9	1.05	0	0.55	5.56
m-ethyl acetophenone	0.88	1.04	0	0.55	5.57
cyclononanone	0.5	0.77	0	0.56	5.58
1-methyl-1-methyl indan	1.02	0.69	0	0.23	5.59
1-cyclohexylbutan-2-one	0.48	0.8	0	0.59	5.6
o-ethyl acetophenone	0.88	1.06	0	0.55	5.61
1-Decanol	0.19	0.42	0.37	0.48	5.63
butyl cycloheptene	0.45	0.26	0	0.2	5.64
1-ethyl 2-propyl cyclohexane	0.45	0.31	0	0.11	5.65
1,5-dodecadiene	0.28	0.24	0	0.19	5.67
1,6-dodecadiene	0.28	0.52	0	0.19	5.67
1,4-dodecadiene	0.28	0.29	0	0.21	5.67
butyl cycloheptane	0.38	0.2	0	0.11	5.67
1,2-dimethyl indan	1.08	0.69	0	0.25	5.69
1,3-dodecadiene	0.32	0.36	0	0.19	5.69
diisopentyl ketone	0.26	0.7	0	0.63	5.69
dodecene	0.23	0.25	0	0.18	5.7
iso-dodecane	0.17	0.12	0	0.12	5.72
1,1-Dimethylindene	1.14	0.94	0	0.24	5.73
2-Undecanone	0.1	0.68	0	0.51	5.73
methyl cyclodecane	0.42	0.22	0	0.12	5.75
pentyl ketone = pentyl pentanone	0.26	0.74	0	0.54	5.76
n-dodecane	0.17	0.13	0	0.11	5.78

tridecyne	0.17	0.13	0	0.11	5.78
ethyl indan	1.02	0.79	0	0.26	5.8
methyl Tetralin	1.06	0.79	0	0.25	5.81
2-methyl Naphthalene	1.3	0.9	0	0.3	5.83
cycloundecene	0.54	0.29	0	0.19	5.85
propyl cyclooctene	0.46	0.27	0	0.2	5.86
1-methyl Naphthalene	1.31	0.93	0	0.29	5.87
hexylbenzene	0.75	0.69	0	0.26	5.88
cyclodecanone	0.51	0.79	0	0.57	5.89
1-Methylene-1,2,3,4-tetrahydronaphthalene	1.15	0.91	0	0.26	5.91
cycloundecane	0.53	0.22	0	0.11	5.91
heptyl cyclopentene	0.45	0.3	0	0.2	5.92
hexyl cyclohexane	0.44	0.29	0	0.12	5.96
1-methyl 2-pentyl benzene	0.76	0.68	0	0.25	5.96
benzyl propyl ketone	0.83	1.06	0	0.57	5.98
hexyl cyclohexene	0.51	0.32	0	0.2	5.99
isohexyl cyclohexane	0.4	0.34	0	0.11	5.99
1-methoxyindan	1.07	1	0.01	0.56	6.02
p-propyl acetophenone	0.89	1.06	0	0.55	6.04
1,6-tridecadiene	0.3	0.3	0	0.22	6.04
1,4-tridecadiene	0.29	0.27	0	0.19	6.05
1,3-tridecadiene	0.33	0.38	0	0.19	6.05
1,5-tridecadiene	0.3	0.31	0	0.21	6.05
o-propyl acetophenone	0.9	1.08	0	0.56	6.09
methyl Decalin	0.72	0.43	0	0.13	6.09
iso-tridecane	0.17	0.13	0	0.13	6.12
tridecene	0.27	0.22	0	0.19	6.12
1-Undecanol	0.18	0.42	0.37	0.48	6.13
1,2-Dimethyl-4-butylbenzene	0.77	0.67	0	0.27	6.13

1-methyl 3-pentyl cyclohexane	0.41	0.33	0	0.1	6.14
tetralone	1.21	1.16	0.01	0.54	6.14
cyclohexylbenzene	0.95	0.72	0	0.23	6.16
Biphenyl	1.22	0.97	0	0.31	6.17
cyclododecene	0.56	0.31	0	0.18	6.17
(2,4-Cyclopentadien-1-ylidenemethyl)benzene	1.18	0.88	0	0.27	6.17
2,6-Dimethylnaphthalene	1.38	0.88	0	0.31	6.22
cycloheptyl-3-butanone	0.45	0.8	0	0.59	6.24
1-methyl 1-pentyl cyclohexane	0.47	0.31	0	0.12	6.24
2-Vinylnaphthalene	1.38	0.95	0	0.29	6.25
1-propyl 2-propyl benzene	0.78	0.66	0	0.25	6.25
1,2-Dimethyl-3-butylbenzene	0.79	0.68	0	0.27	6.25
1-ethyl 2-butyl benzene	0.77	0.66	0	0.25	6.25
propyl indan	1.09	0.81	0.01	0.25	6.26
2-ethyl Naphthalene	1.36	0.94	0	0.29	6.26
cyclododecane	0.55	0.24	0	0.1	6.26
1-methyl 2-pentyl cyclohexane	0.45	0.34	0	0.1	6.26
1-ethyl Naphthalene	1.39	0.92	0	0.29	6.29
n-tridecane	0.19	0.15	0	0.11	6.29
tetradecyne	0.19	0.15	0	0.11	6.29
1-Vinylnaphthalene	1.41	0.96	0	0.29	6.3
heptylbenzene	0.77	0.74	0	0.26	6.31
5-Methyl-1-phenylhexa-1,3,4-triene	0.96	0.87	0	0.26	6.34
1,6-Dimethylnaphthalene	1.4	0.95	0	0.29	6.36
1,2,4-Triethylbenzene	0.81	0.67	0	0.26	6.37
1-ethyl 3-butyl cyclohexane	0.42	0.34	0	0.11	6.37
ethylbutyl cyclohexane	0.49	0.35	0	0.11	6.4
1,2,4-triethyl cyclohexane	0.53	0.44	0	0.13	6.44
butyl cyclooctane	0.41	0.23	0	0.12	6.47

ethyl Tetralin	1.16	0.84	0	0.24	6.48
1,2,3-Triethylbenzene	0.86	0.68	0	0.26	6.48
1,2-Dimethylnaphthalene	1.45	0.99	0	0.3	6.52
ethyl cyclodecane	0.43	0.24	0	0.11	6.57
hexyl ketone	0.27	0.78	0	0.56	6.58
p-butyl acetophenone	0.89	1.09	0	0.56	6.61
1,3-tetradecadiene	0.34	0.47	0	0.23	6.61
1,4-tetradecadiene	0.32	0.39	0	0.23	6.61
1,5-tetradecadiene	0.3	0.32	0	0.23	6.61
1,6-tetradecadiene	0.3	0.31	0	0.24	6.61
octyl cyclopentene	0.48	0.37	0	0.19	6.62
o-butyl acetophenone	0.91	1.11	0	0.57	6.63
Acenaphthene	1.54	1.12	0	0.21	6.64
tetradecene	0.25	0.27	0	0.22	6.66
iso-tetradecane	0.18	0.14	0	0.12	6.66
1,2-dimethyl tetralin	1.26	0.74	0	0.24	6.68
heptyl cyclohexene	0.51	0.38	0	0.19	6.68
1,2,3,4-Tetramethyl-5-ethylbenzene	0.91	0.71	0	0.29	6.69
1,2-Dimethyl-3-pentylbenzene	0.78	0.68	0	0.27	6.7
Acenaphthylene	1.54	1.12	0	0.21	6.71
heptyl cyclohexane	0.44	0.34	0	0.12	6.71
1,5-Dimethyl-1,2,3,4-tetrahydronaphthalene	1.25	0.75	0	0.22	6.72
1-methyl-1-ethyl indan	1.1	0.72	0	0.22	6.72
5,8-Dimethyl-1,2,3,4-tetrahydronaphthalene	1.24	0.8	0	0.22	6.73
n-tetradecane	0.2	0.14	0	0.11	6.74
pentadecyne	0.2	0.14	0	0.11	6.74
1,5-pentadecadiene	0.2	0.14	0	0.11	6.74
1,6-pentadecadiene	0.2	0.14	0	0.11	6.74
1,1-dimethyl tetralin	1.14	0.74	0	0.21	6.75

1,2,3-triethyl cyclohexane	0.6	0.43	0	0.13	6.75
(1Z)-1,2,3-Octatrien-1-ylbenzene	0.95	0.85	0	0.26	6.76
2-methyl Biphenyl	1.38	1.01	0	0.32	6.77
1-methyl 2-hexyl benzene	0.78	0.73	0	0.25	6.78
butyl indan	1.15	0.88	0.01	0.24	6.81
1-methyl 4-hexyl cyclohexane	0.39	0.37	0	0.1	6.85
1-ethyl 2-pentyl benzene	0.81	0.71	0	0.25	6.85
3-methyl Biphenyl	1.38	1.02	0	0.32	6.85
4-methyl Biphenyl	1.37	1.02	0	0.33	6.86
1-propyl 2-butyl benzene	0.82	0.71	0	0.25	6.86
cyclotridecane	0.57	0.27	0	0.1	6.91
Fluorene	1.59	1.06	0	0.25	6.92
cyclotridecene	0.57	0.33	0	0.18	6.95
methylhexyl cyclohexane	0.47	0.38	0	0.12	6.97
ethyl Decalin	0.93	0.48	0	0.13	6.97
1-(3-Buten-1-yl)-1H-indene	1.31	1.05	0	0.3	7.03
2-propyl Naphthalene	1.38	1.08	0	0.3	7.03
3-Methyl-7-phenylhepta-1,3,4-triene	0.88	0.86	0	0.3	7.05
octylbenzene	0.79	0.8	0	0.26	7.06
(1E)-1-Octen-1-ylbenzene	0.89	0.97	0	0.28	7.06
1-propyl Naphthalene	1.43	1.11	0	0.3	7.07
2-Ethyl-7-methylnaphthalene	1.46	0.96	0	0.29	7.08
2-Isopropylnaphthalene	1.46	1.05	0	0.3	7.08
hexamethylbenzene	0.97	0.71	0	0.32	7.09
2-Ethyl-3-methylnaphthalene	1.49	1.03	0	0.3	7.09
2,3,6-Trimethylnaphthalene	1.47	0.97	0	0.31	7.1
(1E)-1-(2-Propen-1-ylidene)-1,2,3,4-tetrahydronaphthalene	1.4	1.06	0	0.26	7.1
4-[(1E)-1-Propen-1-yl]-1,2-dihydronaphthalene	1.4	1.08	0	0.27	7.11

4-Allyl-1,2-dihydronaphthalene	1.39	1.07	0	0.26	7.11
2-Ethyl-6-methylnaphthalene	1.46	0.97	0	0.3	7.11
3-(2-Methyl-propenyl)-1H-indene	1.39	0.98	0	0.25	7.12
1-(Dimethylamino)naphthalene	1.48	1.24	0.01	0.64	7.12
2-Allyl-3-methyl-1H-indene	1.43	1.11	0	0.29	7.14
[(1E,3E)-6-Methyl-1,3,5-heptatrien-1-yl]benzene	0.98	0.92	0	0.27	7.14
3-(3-Buten-2-yl)-1H-indene	1.45	1.07	0.01	0.26	7.14
1-Isopropylnaphthalene	1.51	1.11	0	0.29	7.16
1,6,7-Trimethylnaphthalene	1.5	1.03	0	0.29	7.19
1,1'-(1,2-Ethanediyl)dibenzene	1.35	1.06	0	0.34	7.19
(4-Vinyl-3,5-hexadien-1-yl)benzene	0.93	0.88	0	0.29	7.19
1,2,6-Trimethylnaphthalene	1.49	1.04	0	0.29	7.2
1,2,7-Trimethylnaphthalene	1.49	1.04	0	0.28	7.22
1,3,7-Trimethylnaphthalene	1.47	1.06	0	0.28	7.22
1-Ethyl-8-methylnaphthalene	1.52	1.09	0	0.28	7.23
1,3,6-Trimethylnaphthalene	1.47	1.07	0	0.28	7.24
nonyl cyclopentene	0.51	0.39	0	0.19	7.25
(3E)-1,3,7-Octatrien-2-ylbenzene	1.02	1.03	0	0.31	7.27
1,2-Dimethyl-3-hexylbenzene	0.79	0.71	0	0.27	7.27
1-Benzyl-3-methylbenzene	1.34	1.02	0	0.33	7.28
1-Benzyl-2-methylbenzene	1.37	1.06	0	0.32	7.29
1,1'-(1,1-Ethanediyl)dibenzene	1.41	1.1	0	0.32	7.29
1-Benzyl-4-methylbenzene	1.32	1.05	0	0.33	7.3
2,2'-Dimethylbiphenyl	1.55	1.15	0	0.29	7.31
ethylpentyl cyclohexane	0.52	0.38	0	0.12	7.31
(2-Allyl-1,4-pentadien-1-yl)benzene	1.02	1.05	0	0.31	7.31
2,6-Dimethylbiphenyl	1.55	1.14	0	0.28	7.32
1,4,6-Trimethylnaphthalene	1.48	1.1	0	0.25	7.33
pentyl indan	1.22	0.94	0.01	0.24	7.33

1,4-pentadecadiene	0.31	0.3	0	0.2	7.34
2,4-Dimethylbiphenyl	1.51	1.19	0	0.3	7.34
1-methyl-1-propyl indan	1.16	0.7	0	0.23	7.34
1,3-pentadecadiene	0.35	0.51	0	0.24	7.35
1-[(3E)-1,3,6-Heptatrien-4-yl]-2-methylbenzene	1.11	1.07	0	0.3	7.35
2,3'-Dimethylbiphenyl	1.52	1.16	0	0.3	7.35
2,5-Dimethylbiphenyl	1.52	1.15	0	0.29	7.36
propylbutyl cyclohexane	0.55	0.38	0	0.11	7.36
4-Ethylbiphenyl	1.4	1.19	0	0.33	7.36
3,4-Dimethylbiphenyl	1.5	1.18	0	0.31	7.36
1,2,3-Trimethylnaphthalene	1.5	1.11	0	0.26	7.37
2,3-Dimethylbiphenyl	1.54	1.18	0	0.29	7.37
1,2,5-Trimethylnaphthalene	1.5	1.11	0	0.26	7.38
3-Ethylbiphenyl	1.44	1.21	0	0.33	7.38
1,3,5-Trimethylnaphthalene	1.5	1.09	0	0.26	7.38
1-methyl 2-heptyl benzene	0.84	0.78	0	0.26	7.39
2,4'-Dimethylbiphenyl	1.51	1.17	0	0.3	7.39
octyl cyclohexane	0.48	0.37	0	0.12	7.39
methyl cyclohexylbenzene	1.14	0.85	0	0.25	7.4
3,5-Dimethylbiphenyl	1.51	1.16	0	0.3	7.4
2-Ethylbiphenyl	1.48	1.2	0	0.32	7.4
3,4,4a,9a-Tetrahydrofluorene	1.57	0.9	0	0.24	7.41
3,4,4a,9a-Tetrahydrofluorene	1.57	0.9	0	0.24	7.41
3,3'-Dimethylbiphenyl	1.5	1.18	0	0.3	7.41
1,3,8-Trimethylnaphthalene	1.5	1.1	0	0.24	7.42
3,4'-Dimethylbiphenyl	1.47	1.15	0	0.31	7.42
2-(3-Buten-1-yl)naphthalene	1.44	1.17	0	0.31	7.43
2-Methyl-1-methylene-2-vinylindane	1.38	1.07	0	0.24	7.43
4,4'-Dimethylbiphenyl	1.46	1.13	0	0.32	7.43

1,2,4-Trimethylnaphthalene	1.53	1.12	0	0.25	7.46
pentadecene	0.26	0.3	0	0.23	7.46
1,2,8-Trimethylnaphthalene	1.53	1.12	0	0.26	7.46
propyl Tetralin	1.26	0.98	0	0.24	7.48
2-(2-Methyl-2-propen-1-yl)naphthalene	1.49	1.19	0	0.28	7.49
1-tert-Butyl-4-(2-methylprop-2-en-1-yl)benzene	0.92	0.79	0	0.26	7.5
1-(2-Methyl-2-propen-1-yl)naphthalene	1.55	1.2	0	0.27	7.51
iso-pentadecane	0.2	0.17	0	0.12	7.52
1,4,5-Trimethylnaphthalene	1.53	1.11	0	0.24	7.55
propyl Decalin	1.05	0.61	0	0.13	7.56
octyl cyclohexene	0.53	0.39	0	0.18	7.57
1-Allyl-4-methylene-1,4-dihydronaphthalene	1.57	1.19	0	0.27	7.57
1-ethyl 2-hexyl benzene	0.87	0.74	0	0.25	7.58
n-pentadecane	0.2	0.17	0	0.09	7.59
hexadecyne	0.2	0.17	0	0.09	7.59
1-propyl 2-pentyl benzene	0.9	0.76	0	0.25	7.62
1-butyl 2-butyl benzene	0.9	0.76	0	0.25	7.63
(3-Cyclopentylpropyl)benzene	1	0.86	0	0.25	7.64
[(E)-2-(1-Cyclohexen-1-yl)vinyl]benzene	1.24	1.13	0	0.31	7.67
phenethylcyclohexane	1.07	0.88	0	0.25	7.73
cyclotetradecene	0.59	0.36	0	0.17	7.74
1,1,2-trimethyl-1,2-dihydronaphthalene	1.36	1.02	0	0.24	7.75
2-Butylnaphthalene	1.38	1.23	0	0.31	7.8
methylheptyl cyclohexane	0.54	0.42	0	0.12	7.81
decyl cyclopentene	0.53	0.43	0	0.19	7.81
1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene	1.28	0.82	0	0.2	7.82
1,2,4,5-Tetraethylbenzene	1.08	0.82	0	0.24	7.82
2-sec-Butylnaphthalene	1.5	1.24	0	0.31	7.82
2-Isobutylnaphthalene	1.45	1.19	0	0.3	7.82

(4-Vinyl-3-cyclohexen-1-yl)benzene	1.22	0.94	0	0.26	7.83
1-Butylnaphthalene	1.44	1.24	0	0.31	7.83
1,2,3,4-Tetraethylbenzene	1.11	0.82	0	0.23	7.84
Cyclohexylethylbenzene	1.21	0.91	0	0.24	7.84
1,1,5,6-Tetramethylindane	1.35	0.77	0	0.22	7.84
hexyl cyclooctene	0.55	0.33	0	0.19	7.84
1,2-Dimethyl-3-heptylbenzene	0.8	0.73	0	0.27	7.84
heptyl ketone	0.3	0.8	0	0.57	7.84
cyclotetradecane	0.58	0.29	0	0.1	7.85
hexyl indan	1.28	0.99	0	0.24	7.86
(4,5-Dimethyl-1,4-cyclohexadien-1-yl)benzene	1.42	1.06	0	0.24	7.86
1-(1,5-Cyclohexadien-1-yl)-3,5-dimethylbenzene	1.41	1.12	0	0.26	7.87
1-Isobutylnaphthalene	1.51	1.2	0	0.29	7.87
4-Cyclohexyl-1,2-dimethylbenzene	1.29	0.91	0	0.24	7.87
1,6,8-Trimethyl-1,2,3,4-tetrahydronaphthalene	1.39	0.87	0	0.2	7.88
1,1,4-Trimethyl-1,2,3,4-tetrahydronaphthalene	1.35	0.82	0	0.2	7.88
butyl Tetralin	1.32	1.11	0	0.24	7.89
2,6-Diethylnaphthalene	1.48	1.13	0	0.28	7.9
6-butyltetralin	1.22	1	0	0.25	7.9
2-Methyl-1-propylnaphthalene	1.57	1.18	0	0.27	7.9
1-Methyl-4-propylnaphthalene	1.57	1.22	0	0.28	7.9
1-Methyl-4-(4-methylcyclohexyl)benzene	1.25	0.91	0	0.22	7.9
2-Allyl-3-methyl-1,2-dihydronaphthalene	1.51	1.19	0	0.28	7.91
1-sec-Butylnaphthalene	1.55	1.26	0	0.29	7.92
1,2-Diethylnaphthalene	1.58	1.12	0	0.25	7.93
1-Isobutyl-1,2,3,4-tetrahydronaphthalene	1.41	1.06	0	0.23	7.93
dimethyl cyclohexylbenzene	1.37	0.91	0	0.23	7.94
5-Isobutyl-1,2,3,4-tetrahydronaphthalene	1.39	0.97	0	0.24	7.94
2-Isopropyl-6-methylnaphthalene	1.52	1.12	0	0.29	7.94

1-Methyl-3-(2-phenylethyl)benzene	1.29	1.13	0	0.32	7.95
1,3-Diethylnaphthalene	1.57	1.22	0	0.28	7.96
nonylbenzene	0.85	0.91	0	0.25	7.96
TETRAHYDROANTHRACENE	1.76	1.28	0	0.45	7.96
1-Methyl-2-(2-phenylethyl)benzene	1.32	1.17	0	0.32	7.97
2-tert-butylnaphthalene	1.5	1.18	0	0.27	7.97
1-Methyl-4-(2-phenylethyl)benzene	1.28	1.14	0	0.33	7.98
1-methyl-7-isopropylnaphthalene	1.55	1.1	0	0.27	8
(2,3-Dimethyl-5-methylene-2-cyclopenten-1-yl)benzene	1.52	0.91	0	0.21	8.01
1-Isopropyl-8-methylnaphthalene	1.59	1.1	0	0.25	8.02
1-Isopropyl-4-methylnaphthalene	1.58	1.09	0	0.25	8.02
1-Benzyl-2-ethylbenzene	1.41	1.19	0	0.32	8.03
1,1'-(1,2-Propanediyl)dibenzene	1.37	1.23	0	0.33	8.04
6-tert-Butyltetralin	1.33	0.92	0	0.23	8.04
1,1-DIPHENYLPROPANE	1.48	1.25	0	0.33	8.05
Tetrahydrophenanthrene	1.76	1.28	0	0.44	8.05
3-(3-Buten-2-yl)-2-methyl-1H-indene	1.55	1.06	0	0.22	8.09
hexadecene	0.28	0.31	0	0.22	8.09
1-Benzyl-4-ethylbenzene	1.3	1.18	0	0.33	8.09
2-Propylbiphenyl	1.49	1.32	0	0.32	8.1
1-Methyl-2-(3-methylbenzyl)benzene	1.48	1.11	0	0.3	8.1
4-Benzyl-1,2-dimethylbenzene	1.46	1.17	0	0.31	8.1
2,5-Dimethyldiphenylmethane	1.5	1.11	0	0.3	8.1
1,1'-Methylenebis(3-methylbenzene)	1.41	1.09	0	0.31	8.11
(4,5,5-Trimethyl-1,3-cyclopentadien-1-yl)benzene	1.39	1.18	0	0.23	8.11
2,2',6-Trimethylbiphenyl	1.66	1.18	0	0.26	8.12
1-Methyl-2-(1-phenylethyl)benzene	1.54	1.18	0	0.31	8.12
1,1'-Methylenebis(2-methylbenzene)	1.51	1.12	0	0.3	8.13

1-Methyl-2-(4-methylbenzyl)benzene	1.45	1.1	0	0.3	8.13
1-Methyl-3-(4-methylbenzyl)benzene	1.4	1.11	0	0.31	8.13
1-Benzyl-2,4-dimethylbenzene	1.49	1.17	0	0.3	8.13
2-Isopropylbiphenyl	1.56	1.27	0	0.31	8.13
iso-hexadecane	0.22	0.18	0	0.11	8.13
2-Benzyl-1,3-dimethylbenzene	1.52	1.12	0	0.29	8.13
1,1'-(2,2-Propanediyl)dibenzene	1.42	1.29	0	0.29	8.14
1-propyl 2-hexyl benzene	0.96	0.87	0	0.23	8.14
5,8-Dimethyl-3-vinyl-1,2-dihydronaphthalene	1.55	1.12	0	0.21	8.15
2-(2-Methyl-3-buten-2-yl)-1H-indene	1.43	1.13	0	0.23	8.15
3-Propylbiphenyl	1.43	1.32	0	0.33	8.15
1-Ethyl-1,2-dihydroacenaphthylene	1.74	1.22	0	0.36	8.15
2,4,6-Trimethylbiphenyl	1.64	1.22	0	0.26	8.16
1-butyl 2-pentyl benzene	0.97	0.87	0	0.23	8.16
4-Propylbiphenyl	1.4	1.34	0	0.33	8.16
cyclopentadecene	0.59	0.37	0	0.16	8.17
n-hexadecane	0.22	0.18	0	0.09	8.17
heptadecyne	0.22	0.18	0	0.09	8.17
3-Isopropylbiphenyl	1.49	1.3	0	0.32	8.17
1,1-Diethyl-1,2,3,4-tetrahydronaphthalene	1.35	0.93	0	0.19	8.18
1-Methyl-4-(1-phenylethyl)benzene	1.49	1.1	0	0.31	8.18
1,2,4-Tripropylbenzene	1.05	0.92	0	0.24	8.19
2-Phenyl-1,2,3,4,5,6-hexahydropentalene	1.52	0.99	0	0.24	8.2
1,1'-Methylenebis(4-methylbenzene)	1.37	1.11	0	0.31	8.2
2,3',5-Trimethylbiphenyl	1.6	1.23	0	0.28	8.2
4-Isopropylbiphenyl	1.47	1.32	0	0.33	8.2
1-(4-Penten-1-yl)naphthalene	1.5	1.28	0	0.3	8.2
[5-(3-Buten-1-yl)-1,4-cyclopentadien-1-yl]benzene	1.47	1.25	0	0.27	8.21
1-Methyl-4,9-dihydro-1H-fluorene	1.74	1.18	0	0.29	8.22

nonyl cyclohexene	0.55	0.46	0	0.19	8.23
2-(3-Methyl-3-buten-1-yl)naphthalene	1.46	1.25	0	0.28	8.23
1,3,6,8-Tetramethylnaphthalene	1.59	1.14	0	0.23	8.23
6-Methoxy-1,1-dimethyl-1,2,3,4-tetrahydronaphthalene	1.37	1.14	0.01	0.55	8.23
2,4',5-Trimethylbiphenyl	1.6	1.25	0	0.28	8.23
3,4',5-Trimethylbiphenyl	1.58	1.27	0	0.29	8.25
2,2,5,7-Tetramethyltetralin	1.46	0.9	0	0.21	8.26
1,3,5,7-Tetramethylnaphthalene	1.6	1.15	0	0.23	8.27
1-[(2E)-2-Penten-3-yl]naphthalene	1.64	1.28	0	0.28	8.28
2,3,6,7-Tetramethylnaphthalene	1.59	1.16	0	0.25	8.28
cyclopentadecane	0.59	0.31	0	0.11	8.29
nonyl cyclohexane	0.52	0.44	0	0.12	8.3
1-Cyclopentyl-1H-indene	1.62	1.14	0.01	0.29	8.3
2,4,4'-Trimethylbiphenyl	1.59	1.26	0	0.29	8.3
4-Ethyl-4'-methylbiphenyl	1.48	1.26	0	0.31	8.3
1-(1-Penten-2-yl)naphthalene	1.62	1.32	0	0.29	8.31
2-(4-Penten-2-yl)naphthalene	1.56	1.31	0	0.34	8.31
1,2,4,7-Tetramethylnaphthalene	1.6	1.15	0	0.23	8.32
1,2,3,4,5,6-Hexahydroanthracene	1.67	1.19	0	0.41	8.32
1,4,5,8-Tetramethylnaphthalene	1.62	1.15	0	0.22	8.32
1,2,6,7-Tetramethylnaphthalene	1.6	1.16	0	0.24	8.33
1,3,6,7-Tetramethylnaphthalene	1.59	1.17	0	0.23	8.34
octyl cycloheptane	0.44	0.28	0	0.11	8.35
1,2,3,4-Tetramethylnaphthalene	1.62	1.14	0	0.24	8.35
1,2,3,7-Tetramethylnaphthalene	1.6	1.16	0	0.24	8.35
1,2,5,7-Tetramethylnaphthalene	1.6	1.16	0	0.22	8.36
undecyl cyclopentene	0.54	0.48	0	0.19	8.37
1,4,6,7-Tetramethylnaphthalene	1.6	1.17	0	0.23	8.37

1,1,3,3,5-Pentamethylindane	1.44	0.84	0	0.21	8.38
2-Ethyl-7-methoxy-1-methylnaphthalene	1.61	1.35	0.01	0.55	8.38
heptyl indan	1.34	1.05	0	0.24	8.39
1,2,3,6-Tetramethylnaphthalene	1.59	1.17	0	0.24	8.39
1,2,5,6-Tetramethylnaphthalene	1.6	1.14	0	0.24	8.4
4a,8a,9,9a,10,10a-Hexahydroanthracene	1.64	0.93	0	0.39	8.41
1,2-Dimethyl-3-octylbenzene	0.8	0.75	0	0.27	8.42
1,1,4,4-Tetramethyl-1,2,3,4-tetrahydronaphthalene	1.41	0.88	0	0.18	8.42
decylbenzene	0.92	0.98	0	0.24	8.42
1,2,3,4,4a,10a-Hexahydrophenanthrene	1.71	1.19	0	0.41	8.43
1,4,5,8,9,10-Hexahydroanthracene	1.58	0.83	0	0.33	8.44
1,2,3,9,10,10a-Hexahydrophenanthrene	1.68	1.18	0	0.38	8.44
1,2,3,4,9,10-Hexahydrophenanthrene	1.67	1.21	0	0.37	8.44
isopropyl cyclohexylbenzene	1.42	1.01	0	0.26	8.47
1,1,2,3,3-Pentamethylindane	1.52	0.85	0	0.22	8.48
7-sec-Butyl-1-methylnaphthalene	1.61	1.27	0	0.27	8.49
1-methyl 2-nonyl benzene	0.96	0.94	0	0.24	8.5
butylated hydroxytoluene	1.21	1.14	0.42	0.61	8.53
Pentaethylbenzene	1.27	0.95	0	0.23	8.57
iso-heptadecane	0.22	0.2	0	0.12	8.6
1-pentyl 2-pentyl benzene	1.03	0.99	0	0.22	8.62
8-Isopropyl-2,5-dimethyl-1,2,3,4-tetrahydronaphthalene	1.57	0.98	0	0.21	8.63
(1S,4S)-4-Isopropyl-1,6-dimethyl-1,2,3,4-tetrahydronaphthalene	1.59	0.99	0	0.22	8.63
heptadecene	0.28	0.33	0	0.23	8.64
6-Isopropyl-1,1-dimethyl-1,2,3,4-tetrahydronaphthalene	1.48	0.96	0	0.23	8.65
1-ethyl 2-octyl benzene	0.98	0.93	0	0.22	8.65

decyl cyclohexane	0.55	0.46	0	0.12	8.66
1-propyl 2-heptyl benzene	1.01	0.96	0	0.22	8.66
1-butyl 2-hexyl benzene	1.02	0.98	0	0.22	8.67
Pentyl tetralin	1.45	1.2	0	0.24	8.68
7-Ethyl-1,1,4-trimethyl-1,2,3,4-tetrahydronaphthalene	1.56	0.98	0	0.22	8.71
1-(2,2-Dimethylcyclopropyl)naphthalene	1.63	1.14	0	0.21	8.71
2-Methyl-1,2,3,4-tetrahydrophenanthrene	1.8	1.24	0	0.29	8.72
cyclohexadecene	0.62	0.38	0	0.17	8.75
n-heptadecane	0.22	0.2	0	0.11	8.76
octadecyne	0.22	0.2	0	0.11	8.76
1,2-Dipropylnaphthalene	1.7	1.3	0	0.29	8.81
1-propyl 2-heptyl benzene	1.01	0.96	0	0.22	8.66
1-butyl 2-hexyl benzene	1.02	0.98	0	0.22	8.67
Pentyl tetralin	1.45	1.2	0	0.24	8.68
7-Ethyl-1,1,4-trimethyl-1,2,3,4-tetrahydronaphthalene	1.56	0.98	0	0.22	8.71
1-(2,2-Dimethylcyclopropyl)naphthalene	1.63	1.14	0	0.21	8.71
2-Methyl-1,2,3,4-tetrahydrophenanthrene	1.8	1.24	0	0.29	8.72
cyclohexadecene	0.62	0.38	0	0.17	8.75
n-heptadecane	0.22	0.2	0	0.11	8.76
octadecyne	0.22	0.2	0	0.11	8.76
1,2-Dipropylnaphthalene	1.7	1.3	0	0.29	8.81
1,2-Dipropylnaphthalene	1.7	1.3	0	0.29	8.81

3.2 Application of spreadsheet

The application of the software can be done by distribute the spreadsheet simulation to the student then in the first hour, allow them to practice simulation in GC for the given set of a sample and in the second hour, allow them to simulate GC×GC results for the given kerosene sample in order to optimize the separation result based on the number of separated peaks within

60 min of the separation time then allow the students to vary independent parameters of column length, column name, flow rate, temperature and the separation performance will be measured according to number of separated peaks (P_{app}).

3.3 Monitoring of the optimization skill

The student optimization skills are evaluated based on screen captures of their performance and evaluate their performance. We will monitor their optimization skills based on screen capture of their performance which will be performed within every 10 minutes for 1 hour. Students needed to capture their screens for every 10 minutes for 1 hour to evaluate their performance and the performance was converted into the scores based on the optimized number of separated peaks and the time they spent to obtain these numbers. The faster they obtain the highest number of separated peaks, the higher the score they will get.

After evaluate we will select some students to perform the simulation tests again but with different experiment question, for example students need to find the conditions to separate target compounds with the minimum separation time. Then provide the alternative tests allowing to practice the green aspect.

3.4 Comparison between simulation results with experiments

The experimental results were provided for as proofs to confirm some of the simulation results in GC×GC. This can be performed by comparing the corresponding experimental and simulated results.

3.4.1 Sample preparation

The mixture containing essential oil compound with 131 compounds. Absolute ethanol for dilution of all samples was purchased from Merck, Germany. The sample was diluted 5 times.

3.4.2 GC×GC condition

An Agilent 7890A gas chromatograph hyphenated with an Agilent 7000 QqQMS (Agilent technologies Inc., US) was applied. The MDGC column set employed a ^{1}D nonpolar HP-5 column (30 m × 0.25 mm ID × 0.25 μm; J&W Scientific, US), a ^{2}D polar Innowax column (2.5 m × 0.25 mm (inner diameter, ID) × 0.50 μm (film thickness); J&W Scientific, US), a restrictor column (DFS): 3.2 m × 0.25 mm, Agilent technologies Inc.), a Dean switch (DS, Agilent technologies Inc.), a flame ionization detector (FID) and the mass spectrometer (MS), as previously described

The FID temperature was at 300 °C using hydrogen, air and N2 flow rates of 30, 300 and 20 mL min^{-1}, respectively. MS ion source temperature, electron ionization voltage, and m/z range were set at 230 °C, -70 eV and 30 - 300, respectively. Oven temperature started from 40°C to 240°C with the other conditions differently performed for each figure. For the developed SNAT modulation system, splitters (DFS columns with ID of 0.18 and 0.25 mm and different lengths) and Y-splitters were applied for multiple loop SNAT system. Periodic H/C strategy (with the window of tsamp or $\Delta t_{R,split}$) was performed within every PM. This applied different nsplit and PM, with the relationship of PM = $\Delta t_{R,split} \times n_{split}$. ^{1}D column inlet pressure program started at 12.1 psi and ramped to 19.5, 22.5 and 24.65 psi with the rate of 1.23, 0.60 and 0.43 psi min-1, respectively. The corresponding values for ^{2}D column (or DS) pressure were fixed at 7 psi. After that, the system is replaced from M-SNAT to the single piece design.

CHAPTER IV

RESULTS AND DISCUSSION

4.1 The example of spreadsheet-based program

The developed spreadsheet is illustrated in **Figure 2.** In this program, there are some parameters that can be changed so that the chart area will change too. The parameters that can be change are Column lengths (Cell B3 and C3), Gas flow rate (Cell B5 and C5), Initial temperature(Cell B9), Heat rate(Cell B10), and both Column1 and Column2 name(Cell G1 for column1 M1 for column2) and for column name that can change, the list of column name are listed in the Cell E7 to E22 from nonpolar to highly polar.
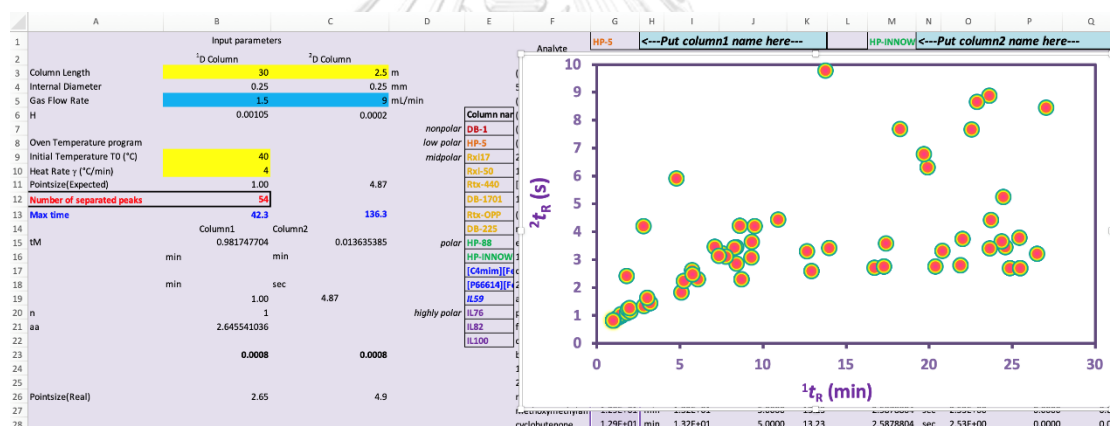
Figure 2. The spreadsheet-based simulation program.

4.2 Application of the spreadsheet in a lecture class for simulation of resultsin GC✕GC

The initial task for students is to investigate performance of the selected column with different pair of columns on kerosene sample separation. This is performed according to the simulated chromatograms and numbers of separated peaks (**Figure 3**).
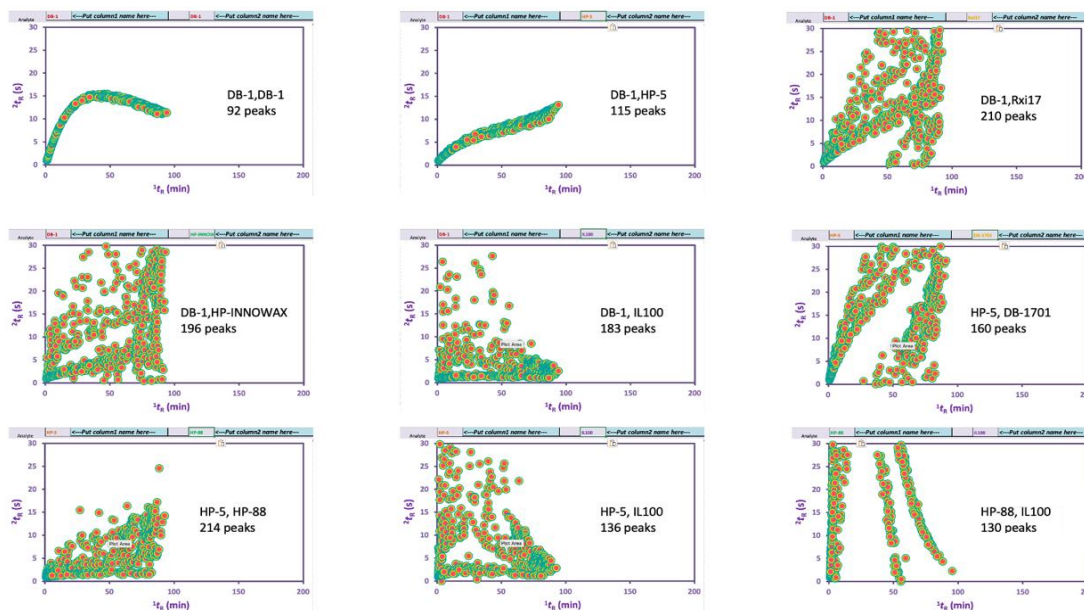
Figure 3. Simulated chromatograms of the kerosene sample containing 641 compounds using different column set.

As shown in **Figure 3**, different pair of columns resulted in the different number of separation patterns and separate peaks. For example, DB-1 pair with DB-1 result in 92 peaks while pairing DB-1 with HP-5 the number of separated peaks change to 115 peaks. The reason different pair resulting in different number of separated peaks is that each pair has different selectivity providing different separation patterns. The separation in GC✕GC is generally expected to be better when the selected column set provides higher degree of selectivity difference between the two columns (Nolvachai et al., 2015b).

4.3 Application of the spreadsheet for column selection and experimental designin GC✕GC

The students were given the software and informed about the software application. They spent about 10 min to get familiar with the software prior to assignment with the goal to separate a mixture within 1 hour of separation time. The students needed to perform column selection by selecting the best column pair from the set of 16 column with different polarities. In addition, they

performed experimental design based on different parameters including column length, flow rate, initial temperature and heat rate. With the starting DB-1✕DB-1 column and the experimental condition shown in **Figure 4A** (before optimization attempt), the obtained result after the optimization attempt is shown in **Figure 4B**. This is especially performed in order to differentiate students with the best optimization skills from the others and to facilitate the scoring process. The word optimization attempt is herein defined as the action to change all the GC✕GC experimental conditions to separate as many peaks as possible within the limited time. Also note that the ideal optimized condition could lead to 235 separated peaks. None of the students in this investigated group could not achieve such condition with the observed average number of separated peaks of 226 ranging from 215 to 234. However, this corresponds to 96% of the peaks that the students could separate average within the short learning time. Since all the students were asked to separate as many peaks as they could, the minimum criteria were based on the average number of separated peaks that they could achieve. Distribution of the student scores (**Figure 4C**) was based on the time they spent and the final separation quality (the number of separated peaks). The student spending the shortest time to achieve the chromatogram similar to that in **Figure 4B.** was scored with the full mark. Based on the performance of students in separating the compound and the time they spent, the average score plotted n **Figure 4C** was around 12 points. This could indicate that most of students are quite good in the simulation. Another thing we observe from this plot is no student score is lower than the half of the full score indicating that students can use this simulation well and some of them are using the simulation proficiently.
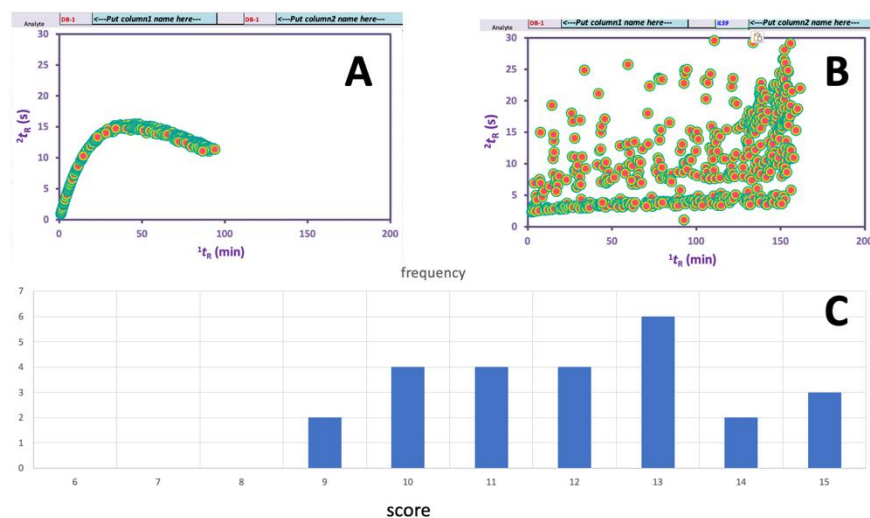
Figure 4. Simulated chromatograms of sample using: (A) a DB-1 and DB-1 column and (B) a DB-1 and IL59 column. (C) The student score distribution.

4.4 Calculation of the score of students

The student scores were calculated based on the numbers of separated peaks they achieved with the time they spent. The resulting scores of each student are shown in **Table 3** for 25 students (no. 1-25) showing the numbers of separated peaks they get in every 5-10 min. The maximum number of separated peaks that each student got within the whole session is also provided in the last column of this Table. The scores were calculated based on three criteria. The first one is the minimum time they spend to get 190 peaks. The next one is the maximum number they get in the first 10 minute. The last one is the actual maximum peaks they got during the whole session. Each of criteria will have maximum score of 5 so the maximum score that a student could gain is 15. The rubrics for the calculation within each criterion are shown in **Tables 4-6**.

Table 3. The separation performance of 25 students obtaining a number of separated peaks in every 5-10 minutes.

Student no.	Number of separated peaks at different test time (minutes)							Max Peaks
	0	5	10	20	30	40	50	
1	65	146	195	213	168	220	217	220
2	65	137	128	138	148	224	228	228
3	65	152	170	182	218	221	234	234
4	65	181	181	192	195	219	226	226
5	65	154	186	181	223	224	228	228
6	65	141	154	149	188	207	226	226
7	65	151	136	155	171	233	233	233
8	65	152	162	154	197	227	227	227
9	65	141	175	183	205	221	234	234
10	65	135	140	197	220	225	226	226
11	65	181	173	167	203	211	233	233
12	65	181	165	180	217	217	224	224
13	65	169	186	216	218	218	218	218
14	65	139	139	152	202	133	224	224
15	65	182	190	193	207	222	232	232
16	65	125	148	171	210	215	226	226
17	65	186	181	202	212	228	234	234
18	65	149	178	189	223	221	229	229
19	65	122	140	171	213	216	219	219
20	65	183	188	200	216	224	228	228
21	65	185	191	202	224	227	228	228
22	65	122	130	131	143	200	222	222
23	65	175	180	194	202	215	215	215
24	65	119	158	179	217	219	220	220
25	65	100	128	159	206	212	226	226

Table 4. Criterion to calculate the student scores based on the time that they spent to achieve their best separation in the simulation.

Score	Time
2.5	none
3	50
3.5	40
4	30
4.5	20
5	10

Table 5. Criterion to calculate the scores based on the number of separated peaks that they achieved within the first 10 min.

Score	Peak range
2	128-138
2.5	138-147
3	147-157
3.5	157-166
4	166-176
4.5	176-185
5	185-195

Table 6. Criterion to calculate the score based on the actual number of maximum peaks they can get in the whole session.

Score	Peak	Range
2	215	218
2.5	218	220
3	220	223
3.5	223	226
4	226	229
4.5	229	231
5	231	234

Details illustrating how to calculate the student's score is provided for the student no. 1 in **Table 3**. The minimum time for this student to get 190 peaks is 10 minutes. According to **Table 4**, this student gained the full 5 points with the first criterion. The second criterion is about the number of maximum peaks this student could get in 10 min. This student could separate 195 peaks within 10 minutes. According to **Table 5**, this is within the range between 185 and 195 getting 5 points under this criterion. The last criterion involves the actual number of separated peaks they got within the whole session. The maximum peaks obtained by this student was 220. According to **Table 6**, this ranges between 220 and 223 corresponding to 3 points from this criterion. The total score of this student is 5+5+3=13 points. This approach was applied to obtain the scores for all the students.

4.5 Test of the optimization skill improvement of students

After the first test above, two students (bachelor and PhD) were asked to perform the new exam with a different sample containing different model compounds. Their performances were monitored and the scores were calculated. **Figures 5 and 6** show the resulting scores the students gained along the exam time. Both student scores were higher than that in the first test even with the different sample. This demonstrated that the developed simulation approach could help students to improve their optimization related skills.
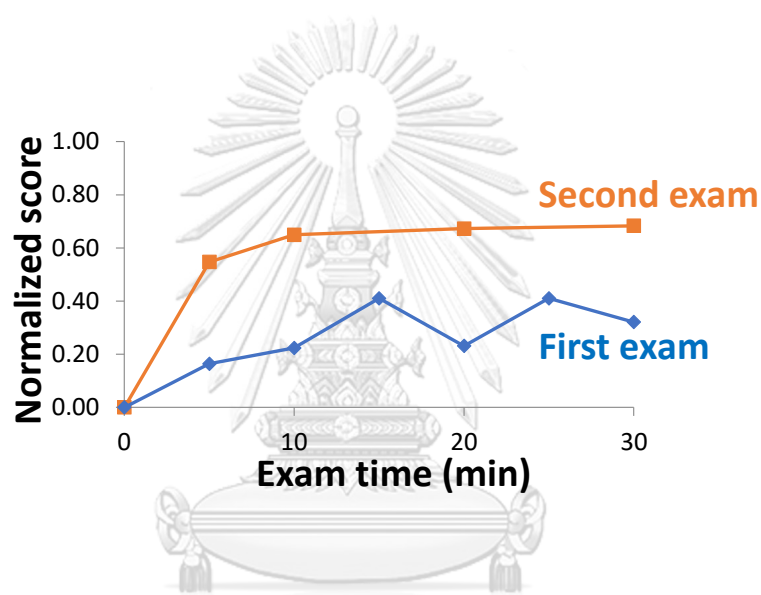
Figure 5. Score vs exam time plots of a Bachelor student in the first and the second exams.
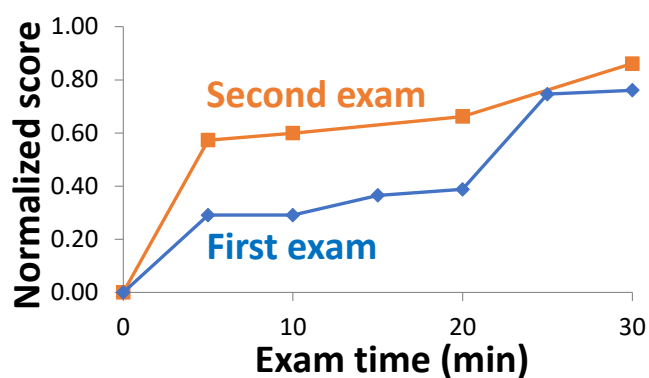
Figure 6. Score vs exam time plots of a PhD student in the first and the second exams.

4.6 Comparison between simulation and actual experiment

Figure 7. shows the comparison between simulated chromatogram and the actual chromatogram. Both chromatograms were obtained using the same experimental condition except for the different temperature increase rates.
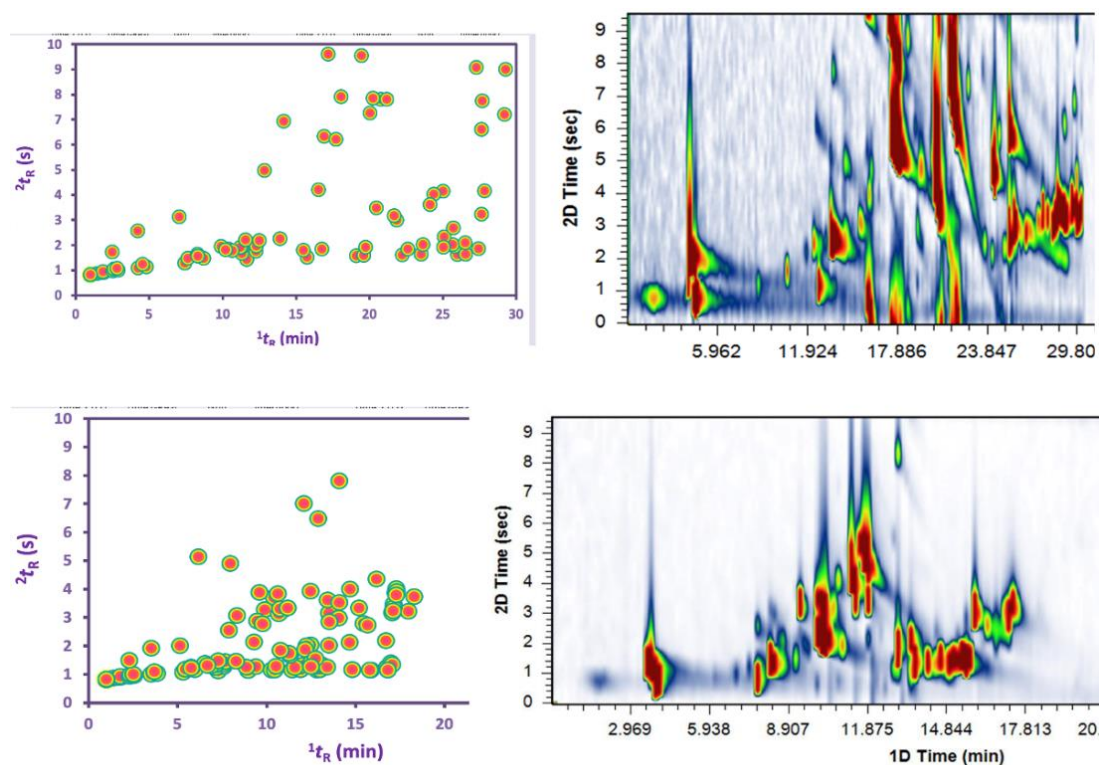
จุฬาลงกรณ์มหาวิทยาลัย
CHULALONGKORN UNIVERSITY

Figure 7. Comparison between the simulation (left column) and actual (right column) chromatograms of an essential oil sample obtained using 4 and 10 $^{\circ}$C/min of the temperature increase rates (top and bottom rows, respectively).

The similarity between the simulated and the actual chromatograms is illustrated with the normalized retention time correlation plots in the **Figure 8.** As expected from the separation timeframes, better correlations were observed in ^{1}D separation with the longer timeframe than the ^{2}D separation. Note that accurate prediction of ^{2}D time requires more advance and lengthier

(several minutes) simulation approaches which are not suitable for the fast (milliseconds) simulation-based learning required in this study.
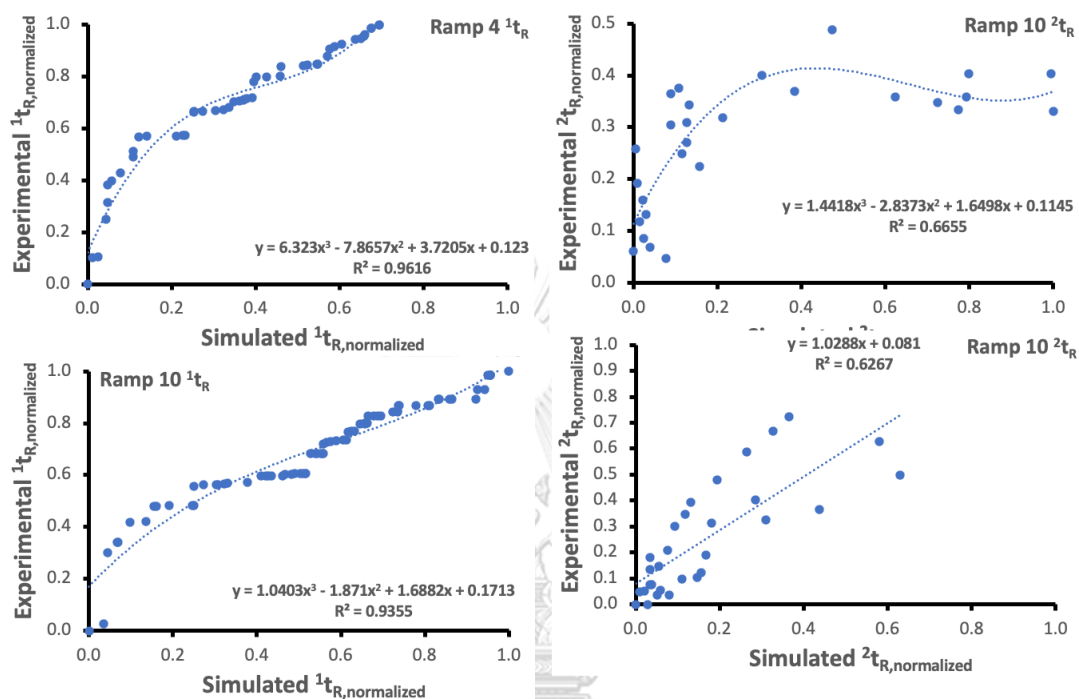
Figure 8. The plot of tendency of simulate chromatogram and actual experiment chromatogram in both ramp 4 and ramp 10.

In addition, the spreadsheets were distributed to 10 volunteers who are not in the field of science. They were given with the starting points using the same column set as that in **Figure 7** but with the condition resulting in poorly separated peaks. Their tasks were to optimize the conditions to result in the same plots as that in **Figure 7**. Their numbers of attempts to reach these optimized conditions were 86, 82, 91, 89, 97, 84, 72, 96, 76, and 94 attempts (pressing enter to see the results in the simulation). We could approximate this as 87 attempts in average until

people outside the field of science could perceive a trial-and-error skill to achieve a separation goal. This can be approximated as ～30 hours of GC×GC experiments.

CHAPTER V

CONCLUSION

The Microsoft Excel spreadsheet-based approach for comprehensive two-dimensional gas chromatography (GC×GC) simulation has been developed. This easily downloadable platform allows student to perform simulation-based practice for column selection and experimental design in GC×GC. The spreadsheet is applicable for simulation of the two-dimensional chromatograms as well as the numbers of separated peaks under different experimental conditions. The application was demonstrated for the optimization of separation of the kerosene containing 641 volatile compounds and an essential oil sample. The sample can be changed by inputting the other set of compounds that are documented in the linear solvation energy relationship (LSER) database. The investigated experimental conditions were mainly column types, initial temperature, column length, heat rate, and gas flow rate. This developed approach can provide the benefit of performing virtual GC×GC within a short amount of time. The application of the spreadsheets allowed the students to practice GC×GC separation with the evident showing improvement of their optimization skills after the practices. This approach could provide knowledge equivalent to that obtained from ∼30 hours of GC×GC experiments for each person, which significantly reduces cost, energy and time consumption.

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