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A TUTORIAL SYSTEM FOR STUDYING
CHROMATOGRAPHY TECHNIQUES

A Project
Presented to the
Faculty of
California State University,
San Bernardino

In Partial Fulfillment
of the Requirements for the Degree
Master of Science
in
Computer Science

by
Hossam Mohamed Hassan

June 2003

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CHROMATOGRAPHY TECHNIQUES


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Hossam Mohamed Hassan

June 2003


Approved by:



Dr. Arturo Concepcion, Chair, Computer
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ABSTRACT

The goal of this project is to use the GTSS (Generic Tutorial System for the Sciences) tools to develop a prototype interactive chromatography simulation with Chrom-Quiz system. This will demonstrate Chrom-Quiz/chromatography integration as a teaching system.

Applets in the GTSS for chemistry will allow the student to conduct multiple experiments without being in the laboratory and without costly equipment and chemicals. The Chromatography applet will provide animation features that show chromatographic separation process, to visually present the concepts of liquid chromatography technique. When embedded in the Chrom-Quiz System, the multiple-choice questions will guide the student to discover the effects of chromatographic variables on separation.

Using the Java technology made it possible to design GTSS/Chrom-Quiz application accessible over the Internet.

ACKNOWLEDGMENTS

The Support of National Science Foundation under the award 9810708 is gratefully acknowledged.

DEDICATION

To My Family

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CHAPTER ONE

INTRODUCTION

1.1 Generic Tutorial System for the Sciences (GTSS) Projects

The Generic Tutorial System for the Sciences (GTSS) provides Java-based interactive simulations to help students in the sciences learn scientific concepts and principles. Most Web sites are plain HTML texts with very little interactivity. Commercial CBT (Computer Based Training) tutorials are very expensive for the student to buy. Dr. Arturo Concepcion, Professor of Computer Science, Dr. Javier Torner, Professor of Physics, and Dr. Charles Stanton, Professor of Mathematics [1] developed the GTSS tutorials not only for students in the sciences but also for educators to use at no charge.

The original GTSS project team focused on developing Java materials for computer science, mathematics and physics, the areas of expertise of its author. The object-oriented approach was used in building the project. The structure of the original GTSS, shown in Fig.1.1, consisted of three layers: core objects, subject engine objects, and application objects.

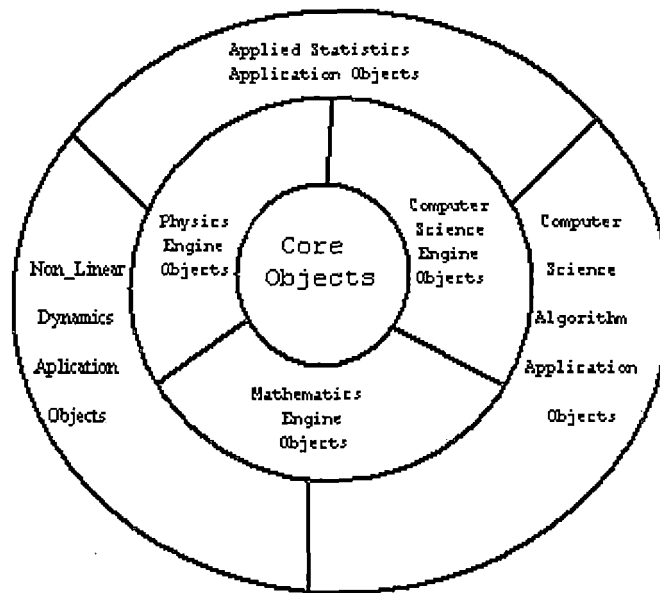


Figure 1. The GTSS Layered Structure

1.1.1 Core Objects

This is a set of primitive reusable objects to build graphical user interfaces (GUI), such as frames, text canvases, buttons, menus, etc. These are the basic building blocks of all of the tutorial systems.

There are seven classes in the core object layer:

1. SGAplet class produces an external frame to run an applet. It initializes a panel and buttons. All the GTSS Applets extend SGAplet.
2. The SGFrame class produces a button panel and a menu bar.
3. The SGMenu class has a private menu labels and menu items.

4. The HsplitPanel class contains two panels in horizontal alignment.
5. The VsplitPanel class contains two panels in vertical alignment.
6. The SplashPanel class extends javax.swing.JFrame, which displays a text string.
7. The SGControlPanel extends javax.swing.JPanel, which constructs a control panel with the button named by ButtonList.

1.1.2 Subject Engine Objects

This set of objects is used as engines to generate specific windows and graphics for a particular science subject. Fig.1.1. shows the subject engine objects for computer science, mathematics, and physics. The engines are built on top of the core objects.

The engine objects include five groups: Computer Science Engines, Mathematics Engines, Statistics Engines, Physics Engines and Utilities.

The Computer Science Engines contains six classes:

1. The Scatter panel class provides a scatter-graph panel to animate sorting algorithms.
2. The Scatter interface class is an interface for accessing the Scatter panel.

3. The sort panel class provides a base panel for sort walks through graphics.
4. The Pseudo code class displays the pseudo code text file for sort walkthroughs.
5. The sort interface class is an interface for accessing sort panel and Pseudo code panels.
6. The sort node class provides an easily enable and the use of visual boxes to represents an array for sorting algorithm demonstration walkthroughs.

The mathematics engines contains 6 classes:

1. Graph panel class plots one or more curves from supplied data, and draws horizontal and vertical axes.
2. The multi graph class is an interface plots multiple curves with graph panel.
3. The GraphPanelIF class is an interface plots single curves with graph panel.
4. The double point class is a wrapper for x, y coordinate. The x and y are double data type.
5. Plot data producer class is used to generate Double points for graph panel.
6. PlotFunctionIF class defines the index Plot function method used by plot data producer.

The Statistics engines contains 8 classes:

1. The Histogram Panel class draws a histogram.
2. The HistogramIF class is an interface for accessing histogram panel.
3. The Histogram adapter class implements HistogramIF.
4. The Histogram data class is used to generate the data needed for Histogram.
5. The Pretty Scale class calculates begin and end points for the scale.
6. The Regress panel class presents regression analysis.
7. The regression calculator class calculates regression coefficients from data.
8. The Data Parser class converts a text file into data.

The Physics engines contains 4 classes:

1. The Rung_Kuttel class computes the next position and velocity of a particle subject to defined acceleration.
2. The Rung_KuttelIF class is an interface for accessing Rung_Kuttel.
3. The Pendulum panel class produces a panel with simple pendulum graphics.

4. The spring panel class produces a panel with simple "spring" graphics.

1.1.3 Application Objects

This set of objects is used to generate the content of windows and graphics for a specific subject. Figure 1.1 shows the specific applications for computer sciences, mathematics, and physics. These objects are implemented on top of their corresponding subjects engine objects and operate through inheritance and polymorphism.

There are five applets in the Computer Science applications: merge sort animation, quick sort animation, bubble sort animation, bubble sort walkthrough and quick sort walkthrough.

Mathematics and statistics have five applets lissajous curve, central limit theorem, bivariate normal simulation, data analysis histograms and regression applets.

Physics has three applets oscillator demo, logistic map, and bifurcation applets.

1.2 Recent Projects

1.2.1 Chemistry Engine Object

In winter 2001 Thomas Gummo [2], graduate student in computer science department, added chemistry objects to

the GTSS project. Dr. Kimberley Cousins, an Associate Professor of Chemistry at CSUSB, and Dr. Arturo Concepcion, Professor of Computer Science, supervised this Master's Project (see Figure 1.2.).

The new application object, An On-Line Acid Base Titration Applet in the GTSS Project, includes a chemical applet for GTSS. The titration applet demonstrates acid base titration by allowing the students to perform virtual titration with acids, and bases, without being in the laboratory and without costly equipment and chemicals.

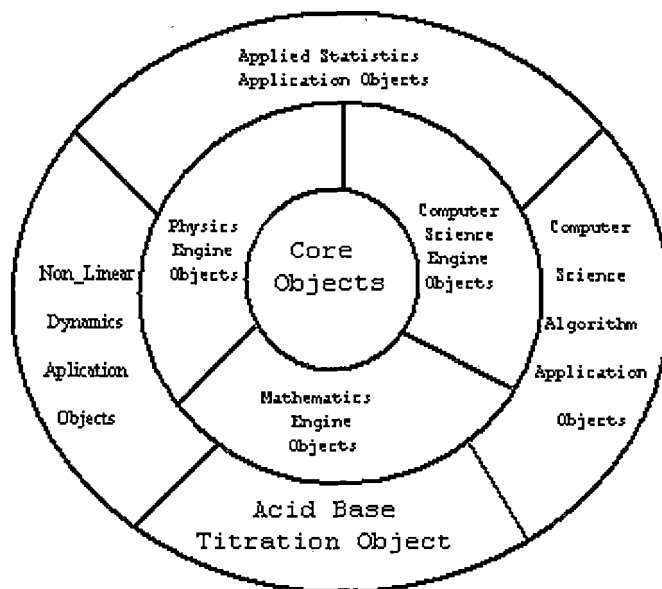


Figure 2. Acid Base Titration Object

1.2.2 Web-based Interactive Self-Evaluation System Project

In Fall 2000 Supachai Praritsantik [3], graduate student in the computer science department, designed the "Web-based Interactive Self-Evaluation System" and analysis of the sorting algorithms in the GTSS project. Dr. Arturo Concepcion, Professor of Computer Science, supervised his Master's Project. The goal of this Master's project was to provide a Web-based interactive exercise for computer science students. WISE provides instructors with tools to create exercises. The students can evaluate their knowledge for analysis of sorting algorithms, using questions designed by their instructor. GTSS-WISE was designed to be accessed through the Internet.

1.3 Chromatography Engine Object

This master's project adds a new application engine to the GTSS structure. The chromatography engine generates animation for a specific chromatography technique. This engine will be used to build the column chromatography applet. The same engine can be reused to build applets for different separation techniques in the future.

1.4 Chromatography Quiz System

This master's project will expand the WISE project, by making specific test questions for the column chromatography technique. GTSS/Chrom-Quiz will provide tools to create exercises for chemistry students at CSUSB. Also, students will be evaluated of their understanding by taking quizzes through Chrom-Quiz.

1.5 Document Organization

Chapter two presents the software requirement specifications for the GTSS and Chrom-Quiz system. Also, the scope of the project is presented.

In Chapter three we illustrate the design of the Chromatography core engine with GTSS structure. Also, the design of the Chrom-Quiz component is explained. In chapters four and five the maintenance and testing of the GTSS and Chrom-Quiz system are discussed. Chapter six outlines the conclusions and the future directions of the GTSS/Chrom-Quiz System.

CHAPTER TWO
SOFTWARE REQUIREMENTS
SPECIFICATION

2.1 Introduction

2.1.1 Purpose of the Project

The purpose of this project is to use GTSS tools to develop a prototype interactive chromatography simulation with the Chrom-Quiz system. This will demonstrate Chrom-Quiz/chromatography integration as a teaching system.

Applets in the GTSS for chemistry will allow the student to conduct multiple experiments without being in the laboratory and without costly equipment and chemicals. The Chromatography applet will provide animation features that show chromatographic separation process, to visually present the concepts of liquid chromatography technique. When embedded in the Chrom-Quiz System, the multiple-choice questions will guide the student to discover the effects of chromatographic variables on separation.

2.1.2 Scope of Project

This project adds new programs to an existing Java system that can be used any way on the World Wide Web.

Java is the ideal language for distributing executable programs via the World Wide Web. Java is a general-purpose language for developing programs that are easily usable and portable across different platforms. This master's projects will include a chromatography simulation in chemistry for GTSS. The Chromatography applet is developed and enhanced by adding classes to the core objects and engine packages. Chemistry is included in the GTSS package as one of the engines, with its own set of applets. Also, Chrom-Quiz System provides tools to create exercises and to evaluate student learning about chromatographic separation process. Column chromatography is commonly used for the separation of chemical compounds. Separation depends on the basic experimental parameters such as packing identity, solvent polarity and pressure. The chemical applet will be interactive. The applet allows students to rapidly conduct multiple simulations of experiments that would normally not be possible due to time, expense and location. Students choose the materials to be separated and the solvent system used for the separation.

2.1.3 Definitions, Acronyms, and Abbreviations

Table 1. Definitions

Algorithm	A set of steps defined such that when they are followed in a specific order, a task is accomplished.
Animation	x-y coordinate mapped representations of data to be operated on by an algorithm. Playing the animation shows, in x-y coordinates, the effects of the algorithm on a static set of test data.
Application Objects	Application objects are implemented on top of their corresponding subjects engine objects and through inheritance and polymorphism.
Browser	A program capable of retrieving HTML documents that includes references to images and Java rendering it into a user-readable document.
Chromatography	It is a broad range of physical methods used to separate and to analyze complex mixtures. The components to be separated are distributed between two phases: a <i>stationary phase</i> and a <i>mobile phase</i> , which percolates across the stationary phase. Chromatography can purify practically any soluble or volatile substance if the right stationary phase, mobile phase, and operating conditions are employed.
Core Objects	A set of reusable objects that is used to build graphical user interface such as frames, buttons, menus, etc.
GTSS	Generic Tutorial System for the Sciences.

GUI	Graphical User Interface. The graphical representation of physical or pseudo-physical objects (such as buttons, trees, and lists) that allow the user to direct the flow of the program through the use of a mouse or other pointing device.
HTML	Hypertext Markup Language. A language that describes the formatting of text inside a browser.
Java	An object-oriented language developed by Sun Microsystems. Java programs are capable of running on most popular computer platforms without the need for recompilation.
JAKARTA-TOMCAT	Tomcat 1.4 is JSP & Servlets server. Tomcat will receive request from a client, execute JSP commands and respond back to client.
JDK	Java Developer's Kit is a Java development environment. Sun Microsystems has supplied a series of that included tools for compiling and testing Java applets and applications. This project uses JDK1.3.
JDBC- Java Database Connectivity	JDBC technology is an Application Programming Interface that lets you access virtually any tabular data source from the Java programming language. It helps Java program to communicate, query and update databases. JDBC needs a JDBC driver as a connector (pipe) between Java programs and databases.
JSP-Java Server Pages	JSP is a Java-based technology that simplifies the process of developing dynamic web sites. JSP is also a type of server-side scripting language.
Servlets	Servlets are the Java platform technology of choice for extending and enhancing Web servers. Servlets provide a component-based, platform-independent method for building Web-based applications

Swing Library	Java Foundation classes (JFC) implements a set of GUI, Graphical user interface, and components.
Subject Engine Objects	The subject engine, which is build on the top of the core objects, will support the generation of windows and graphics for the particular science subject.
Tutorial	Refers to the software package seen by the student, containing scientific simulations
Kow	Concentration ratio of octanol and water
Nsat	Number of molecules in stationary phase
Nmobil	Number of molecules in the mobil phase

2.2 Overall Project Description

2.2.1 Product Perspective

2.2.1.1 System Interfaces. GTSS/Chrom-Quiz system deployment consists of two parts:(1) GTSS/Chrom-Quiz Web server, and (2) the client. The Web server handles any requests from different platforms using TCP/IP protocol. The Chrom-Quiz WEB server contain three layers (1) GTSS for Chromatography applet, (2) Chrom-Quiz Web application, and (3) Mysql database server. These three layers of applications communicate with each other and respond to requests by the client. Chrom-Quiz is running in different platforms (see Figure 3).

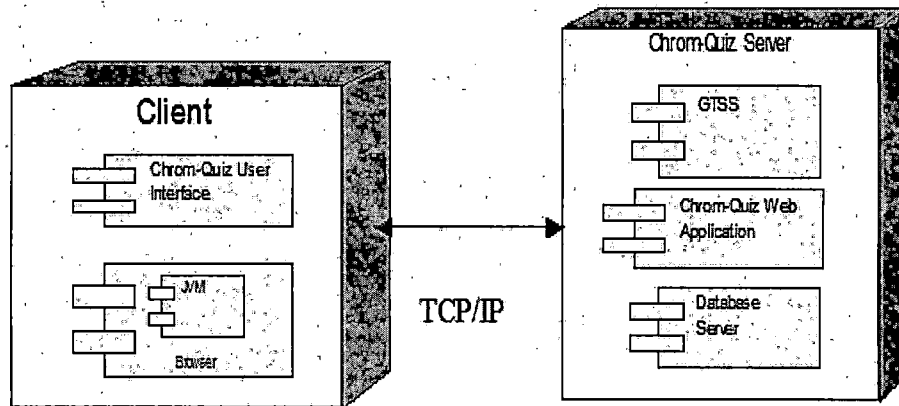


Figure 3. GTSS/Chrom-Quiz Deployment Diagram

2.2.1.2 User Interfaces. Users access the GTSS/Chrom-Quiz through login page. The login page will be entry point for the Chrom-Quiz System. At the login page, users have to enter the userId, password, and select login type. A student can create a new account to access Chrom-Quiz. Users can retrieve their password by accessing the "forget password" page. In the Chrom-Quiz system, there will three types of pages: Instructor page, Student page, and Administrator page. The instructor interfaces welcome page links to different tasks on Chrom-Quiz system. By using those links, the instructor can add new questions and update old questions. Also the instructor can keep track of the students by viewing the student information link. The Instructor can manage the

student information in the Chrom-Quiz database system. The student welcome page is linked to different tasks on Chrom-Quiz system. Students can access the "read about chromatography" link to increase their knowledge before taking the Chromatography quiz. Students can link to the start chromatography quiz question. Students will take the quiz and run the Chromatography simulation applet at the same time in separated windows.

The administrator welcome page is linked to different tasks on Chrom-Quiz system. By using those links, the administrator can manage the student and instructor accounts. The administrator can use create a new account link to add a new instructor account to the Chrom-Quiz database. Also, the administrator can delete students' and instructors' accounts to maintain the Chrom-quiz database system.

2.2.1.3 Hardware Interface. This project was written and tested on the AMD Processor. The system specifications are following:

- Processor type AMD-Athlon 700 Mhz
- Memory 128 MB
- Video Memory 32 MB
- Modem Modem Blaster 56k

2.2.1.4 Software Interface.

- Operating system Windows 2000 professional
- Internet Explorer 6.0
- Jakarta-Tomcat server 4.0
- Java Software development kit (Java 2 platform)
- Mysql database server
- Ideal browser Internet explorer (6.0), Netscape Navigator (6.0) or any browser that has a Java virtual machine.

2.2.1.5 Communication Interface. The GTSS/Chrom-Quiz system can be accessed from a personal computer with Internet access, i.e. modem or DSL cable connection. The GTSS simulation and WISE application server make a complete tutorial for teaching chromatography.

2.2.2 Product Functions

The GTSS/Chrom-Quiz system consists of three levels: student level, instructor level, and administrator level. Figure 4. shows a use case diagram, which describes the information flow of the GTSS/Chrom-Quiz Web application.

1. Chromatography Simulation: This tutorial represents interactive column chromatography as a separation technique.

2. Chromatography Quiz system(Chrom-Quiz): This tool allows the instructors to create interactive exercises in the area of liquid chromatography to make sure that the students understand the concepts of the separation technique. Also, it will help the students to practice and enhance their knowledge about chromatography. Students may repeat the Chrom-Quiz as many times as they wish.

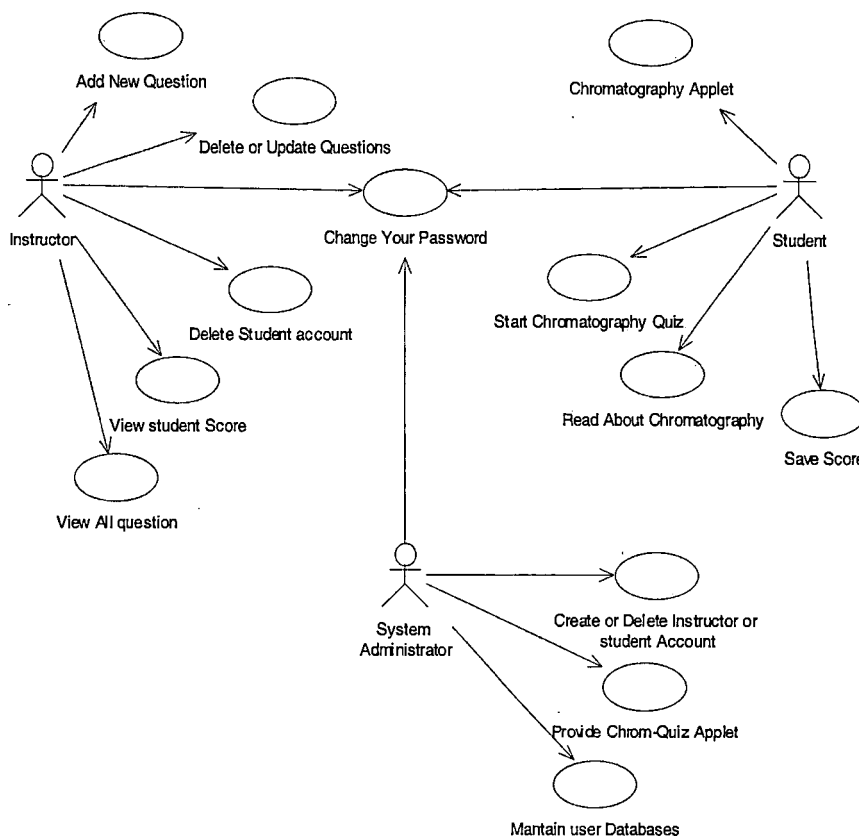


Figure 4. Use Case Diagram for GTSS-Chrom-Quiz System

2.2.2.1 Instructor Level. The instructor will be able to create, edit and delete chromatography questions as shown in Figure 4. The instructor can keep track of the students by accessing the student information, including quiz results saved. Also, the instructor can delete a student account to manage the database without going to the administrator level.

2.2.2.2 Student Level. To access Chrom-Quiz system, student can create new account by accessing the Chrom-Quiz page. Each student will use his userID and his password to access to the Chrom-Quiz System. If the student forgets his password to access the Chrom-Quiz, he can retrieve his password by using "forget password" page. But if he forgets his userID, he has to contact with his instructor to access his account. The student will be able to run the tutorial applet as shown in Figure 4, as often as he wants, before and while answering the questions. If the student does not answer all the questions correctly, he can go back and study the chromatography tutorial and Chromatography applet, and re-take the quiz. Student can save his score to the Chrom-Quiz database system.

2.2.2.3 Administrator Level. The system administrator will be responsible for maintaining the overall GTSS and Chrom-Quiz projects as shown in Figure 4. Only the

administrator can create an instructor account for the WISE system. Also, the administrator will resolve technical problems in the GTSS and Chrom-Quiz system.

2.2.3 System Analysis and Requirements

The GTSS and Chrom-Quiz system depends on several components: a) Apache-Tomcat as servlet container, b) Java Server pages (JSP), c) Java DataBase Connectivity driver (JDBC), d) MYSQL as database server. The components were chosen to integrate a stand-alone GTSS applet into the GTSS and Chrom-Quiz system as described below:

- (a) Apache-Tomcat is the servlet container that is used in the implementation of the Java Servlet and Java Server Pages technologies. We successfully updated the Server from Tomcat 3.2 to 4.0. Tomcat 4 implements the Servlet 2.3 and Java Server Pages 1.2 specifications from Java Software, and includes many features that make it powerful for developing a dynamic web applications and web services. Also, Apache-Tomcat is a free product under General Public License.
- (b) JSP is an extension of Java Technology used to create GTSS. JSP shares the characteristics of Java technology "Write Once, Run Anywhere", and

this is an ideal scripting language to create a web-based interactive self-evaluation system. Another important benefit is the ability to embed reusable components such as Java Beans and Enterprise Java Beans, which can be reused in any number of Java Server Pages. The Chrom-Quiz system has many interactive pages, making JSP an ideal solution.

- (c) Java Database Connectivity (JDBC) driver connects between the Java application and database server (MYSQL). The code for the JDBC is written using pure Java language making its access to the database faster than any other driver.
- (d) Mysql is one of the most popular database servers in the market. It is free product for many platforms including Windows NT, 98, 2000, Linux. MySql is easy to use and easy to maintain. Mysql is a very fast engine and will not affect the speed of the server.

2.2.4 User Characteristics

The GTSS/Chrom-Quiz system requires that users know how to connect to the Internet and how to use a modern Web browser. The intended users will be college chemistry

professors, and their students. This level of user will have experience many basic software programs, and access to lecture and textbook background material in chromatography.

2.3 Software Specific Requirements

2.3.1 External Interface

2.3.1.1 Authorization. The login page for Chrom-Quiz System is shown in Figure 5. Users have to type the userID, password, and select the login type (Student, Instructor, Or Admin). This page will determine the path of the Chrom-Quiz Application.

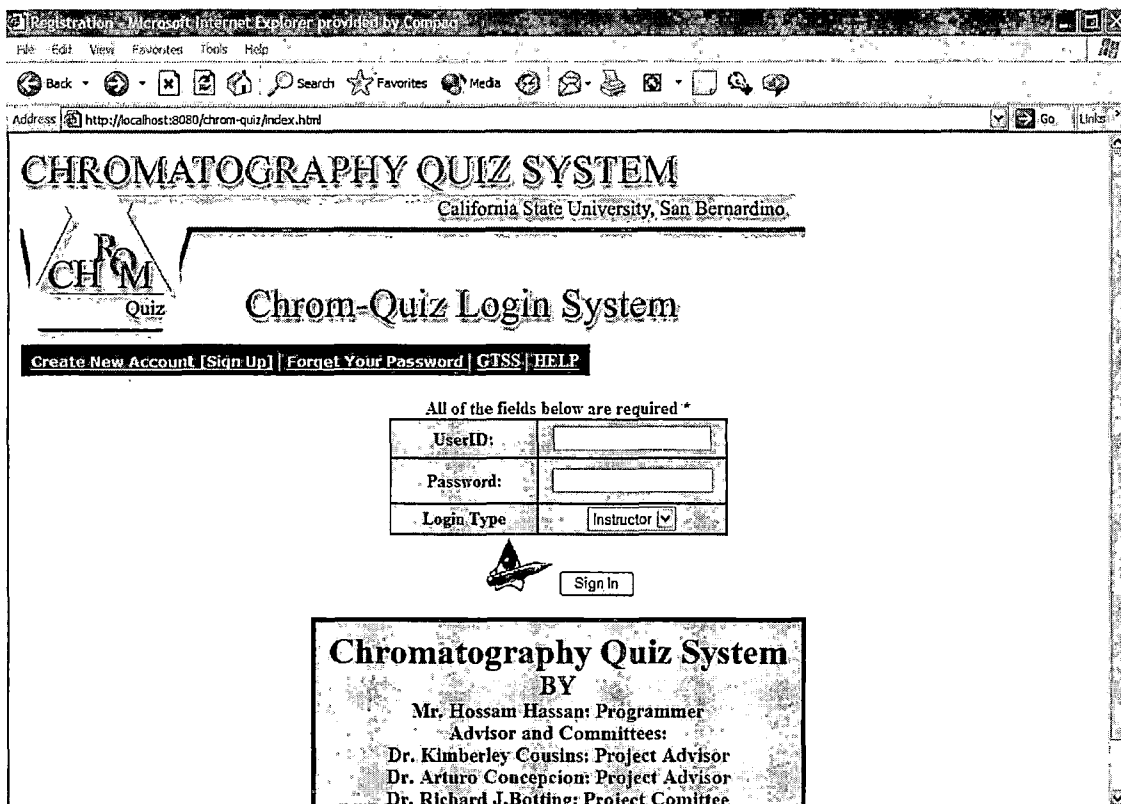


Figure 5. Login Page

2.3.1.2 Create New Student Account. This page will be for the students who are using the Chrom-Quiz system for the first time (see Figure 6). After they fill out the required information, they can access the Chrom-Quiz system.

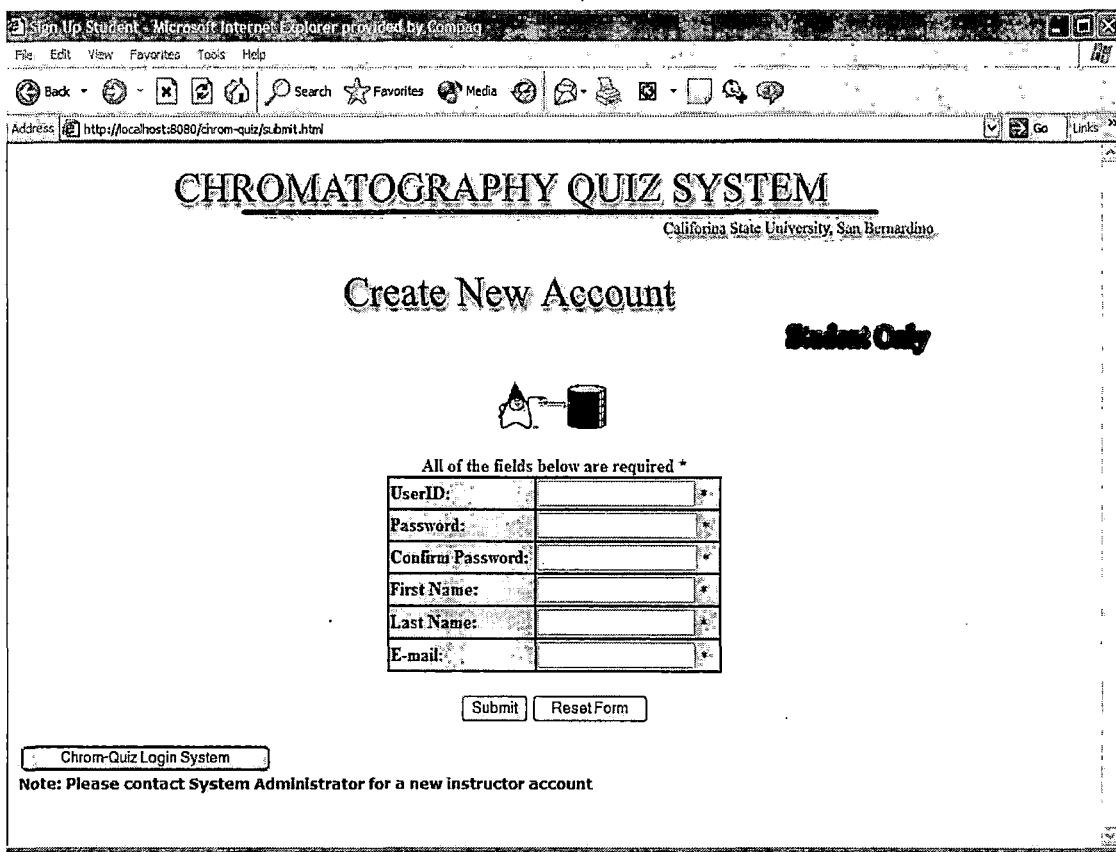


Figure 6. Signup Students

2.3.1.3 Forgot Your Password Page. This page will be for users who forget their password (see Figure 7). Users will fill out the required information and the Chrom-Quiz system will send their password by e-mail.

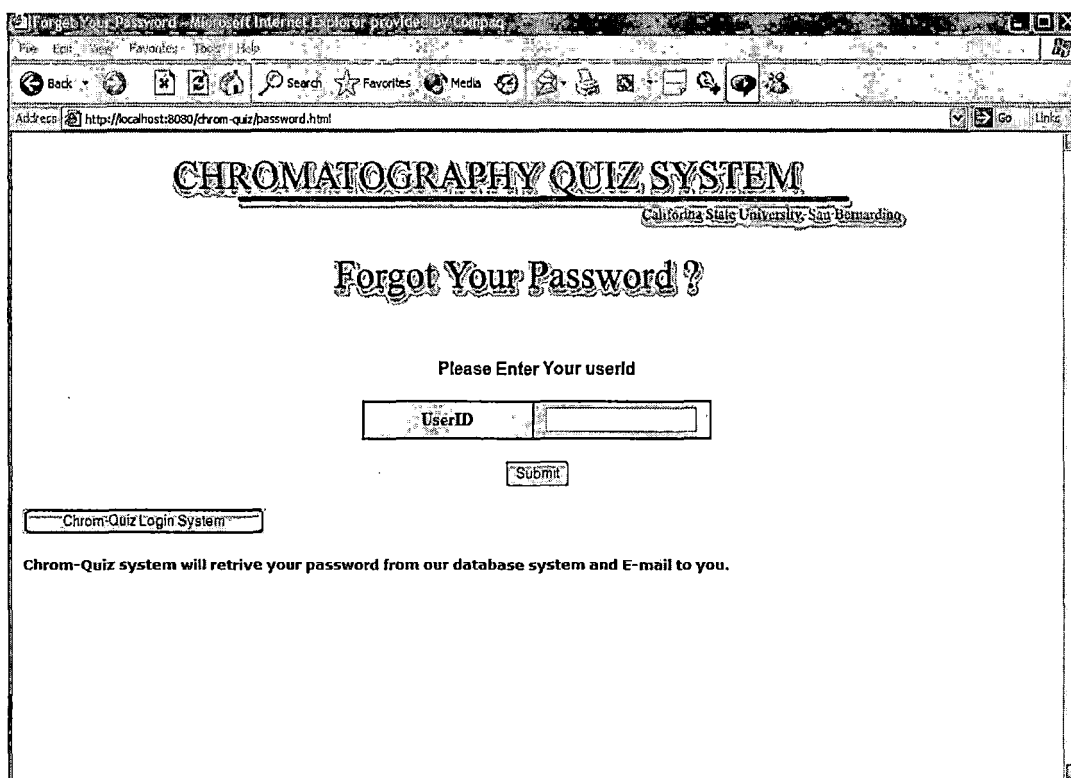


Figure 7. Forgot Your Password Page

2.3.1.4 Instructor Menu. The instructor welcome page links to different tasks on Chrom-Quiz system (see Figure 8). "Add New Question" will allow the instructor to create a new question and save it on Chrom-Quiz database. "Delete question" and "update question" links will let the instructor change the existing questions on in the Chrom-Quiz database. The instructor can access the student information through "View student information" link. Also, Instructor can change his/her password by using the "Change Password" link.

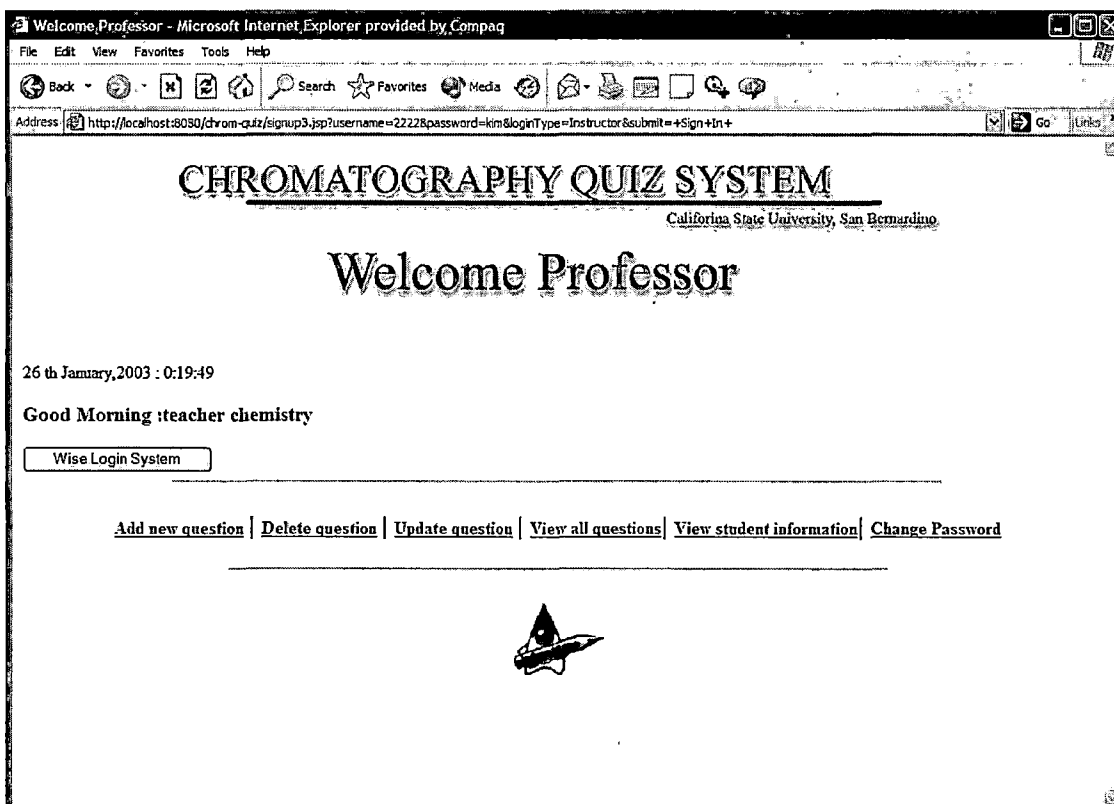


Figure 8. Instructor Welcome Page

2.3.1.5 Add New Question Page. This page will allow the instructor to add a new question to Chrom-Quiz system (see Figure 9). The Instructor will fill out all of the required information and click on the "submit" button. The Chrom-Quiz system will add the information into the database. The instructor can use the "Reset" button to clear page information. Also, the instructor can navigate through the link menu on the bottom of the page.

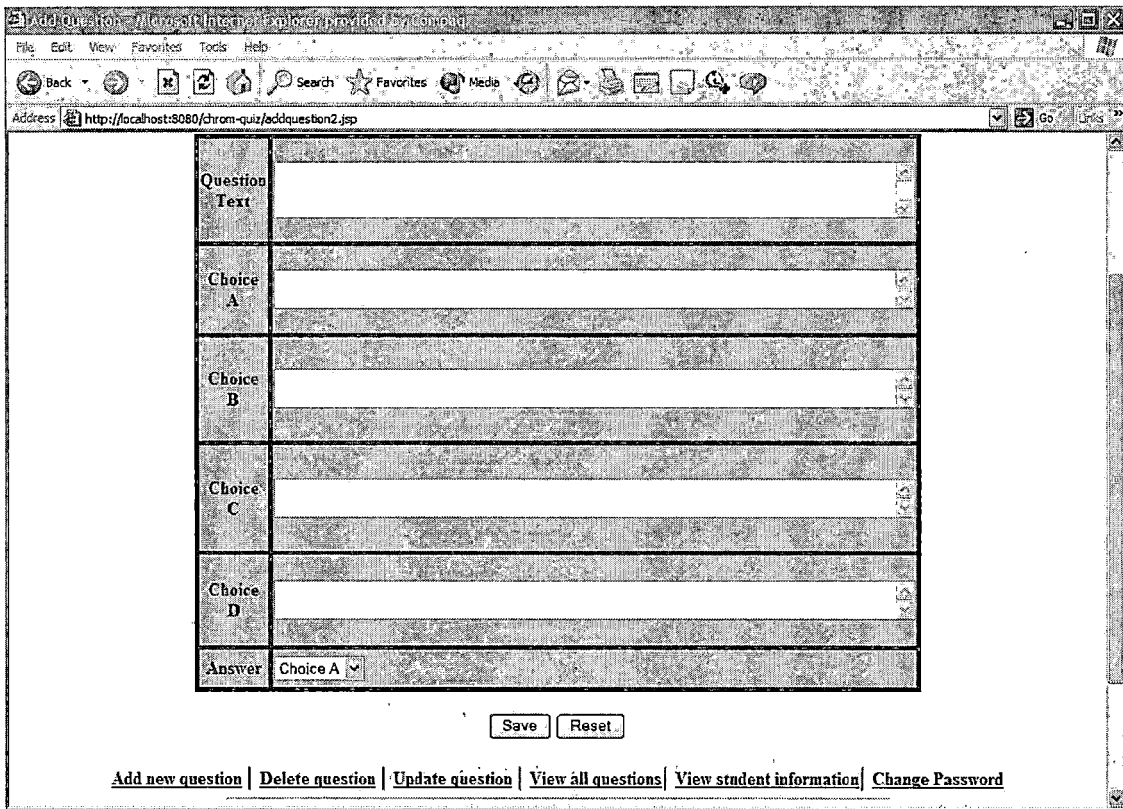


Figure 9. Add New Questions.

2.3.1.6 Delete Or Update Question Page. This page will allow the instructor to delete or update old questions on WISE system (see Figure 10). If the instructor clicks on the "Delete" button, the Chrom-Quiz system will delete this question from the database. Also, the instructor can update the old questions by using the "Update" button. The instructor can navigate through the link menu on the bottom of the page.

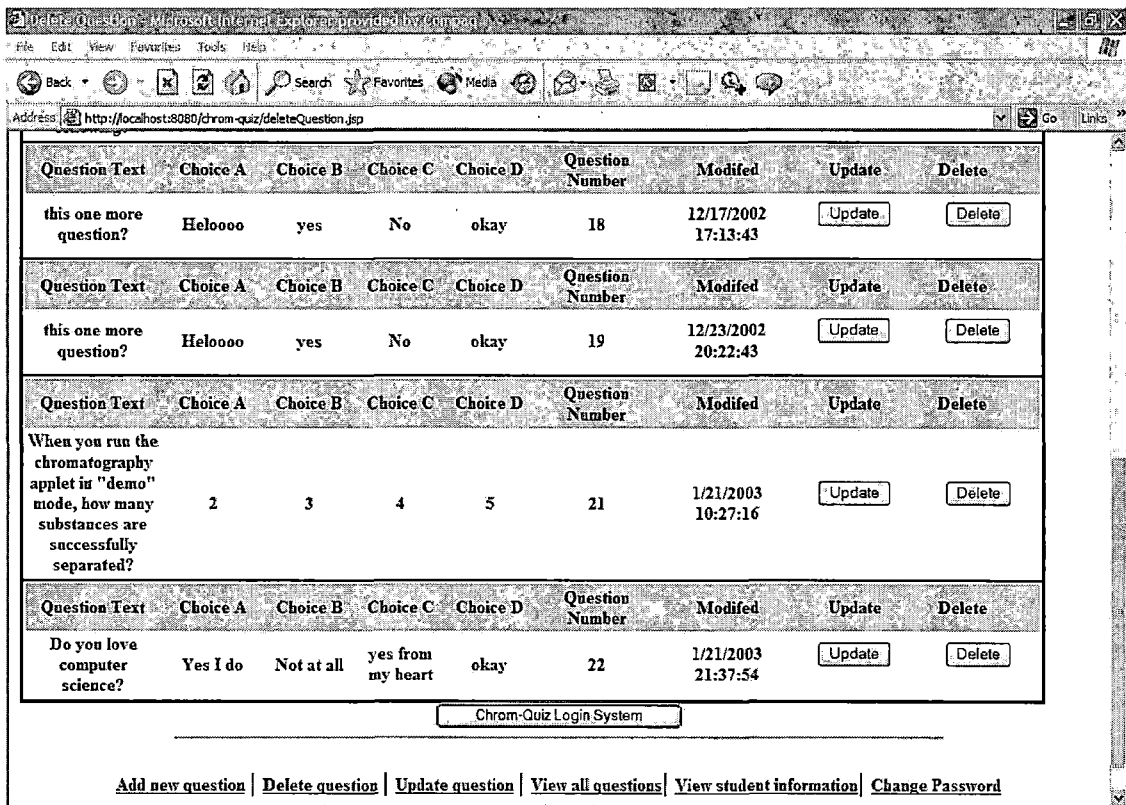


Figure 10. Delete Or Update Question

2.3.1.7 View Student Information Page. This page allows the instructor to access the student information (see Figure 11). Also, the instructor can delete a student account to manage the database without going to the administrator level.

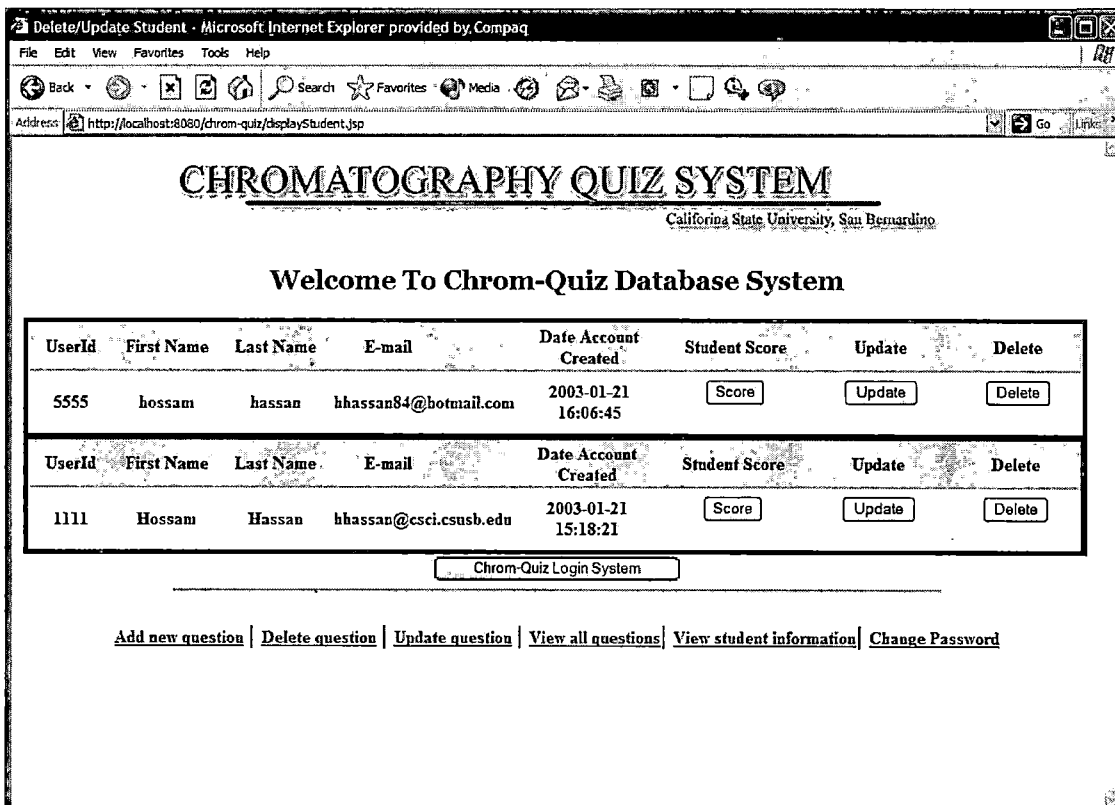


Figure 11. View Student Information

2.3.1.8 Change Instructor Information. This page will allow the instructor to change his personal information (see Figure 12).

2.3.1.9 Student Menu. The student welcome page will link to different tasks on Chrom-Quiz system (see Figure 13). If the student clicks on "Start Chromatography Questions" button, the exercise questions and the chromatography applet will appear on two different

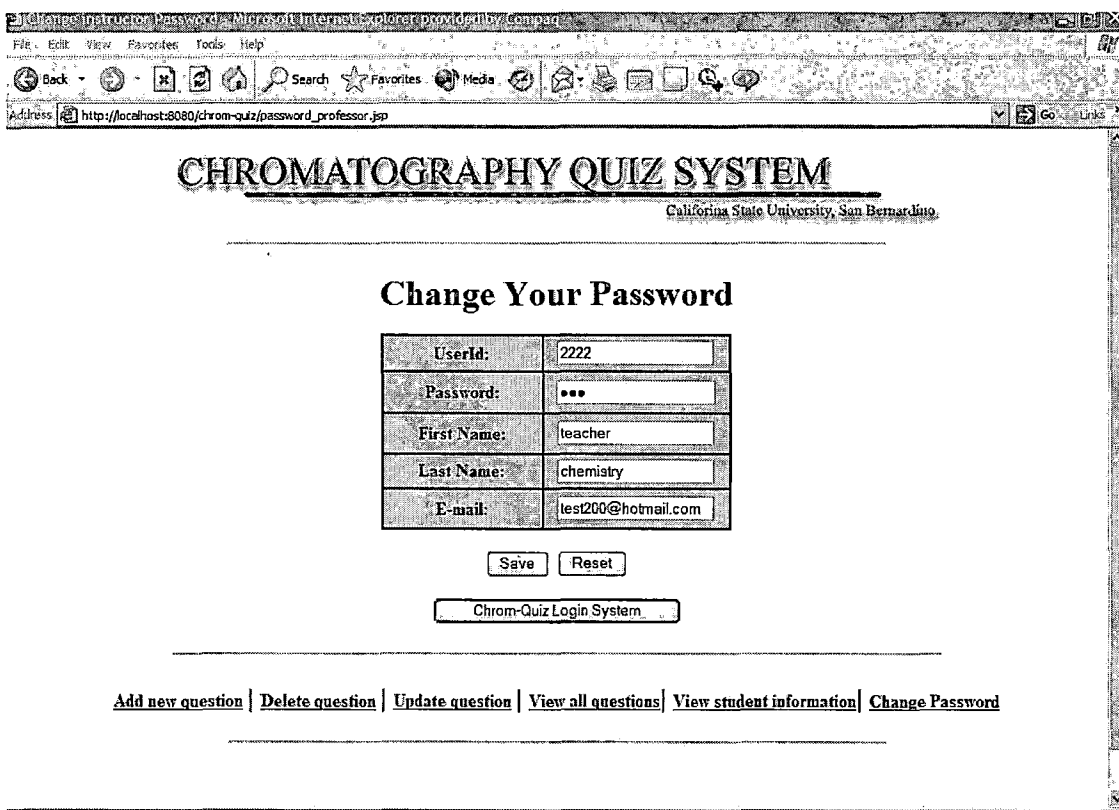


Figure 12. Change Instructor Information

screens. The "Read about Chromatography" button will give a tutorial about the liquid chromatography technique. If the Student clicks on the "Liquid Chromatography Applet", GTSS for liquid chromatography simulation will appear in a new window. Also, if the java plugin does not exist in the student browser, the Chrom-Quiz system will redirect the page to Sun company to install Java plugin.

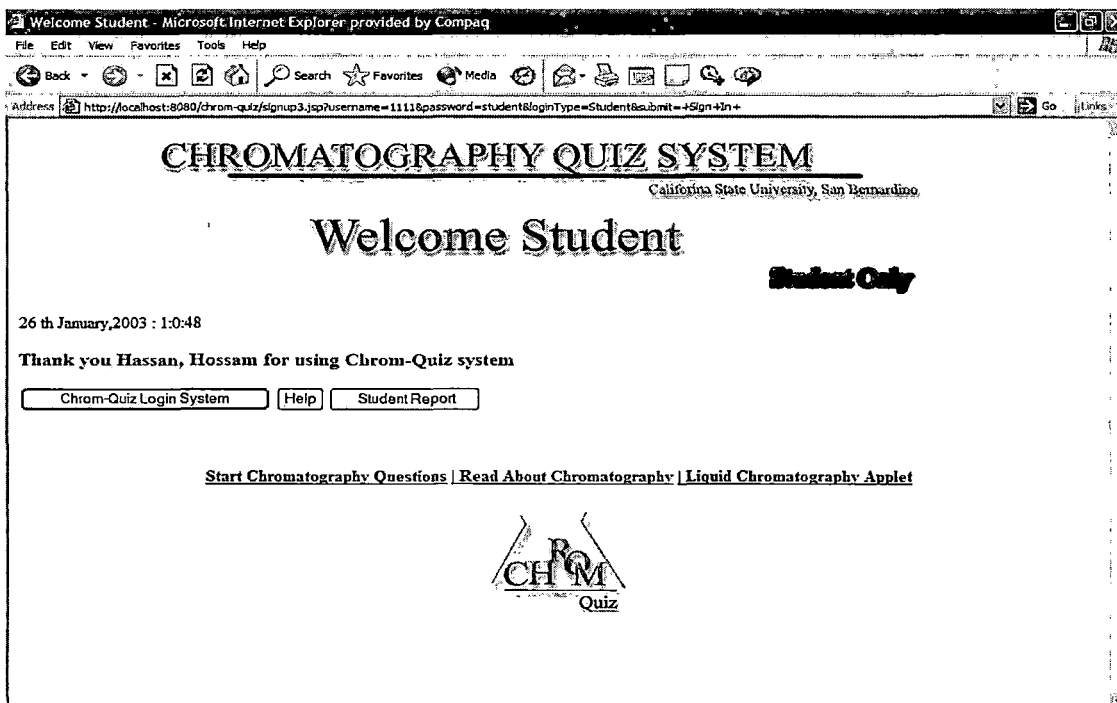


Figure 13. Welcome Student Page

2.3.1.10 Liquid Chromatography Applet. The student can access the chromatography simulation applet from GTSS home page or within the Chrom-Quiz system. The main applet frame is divided into two panels split vertically and a menu bar (see Figure 14). Left panel will show the animation of the compounds that the user has selected as they pass through a column. The right panel is an x-y plot: time is shown on the x-axis and intensity of signal from compounds exiting the column, is shown on the y-axis.

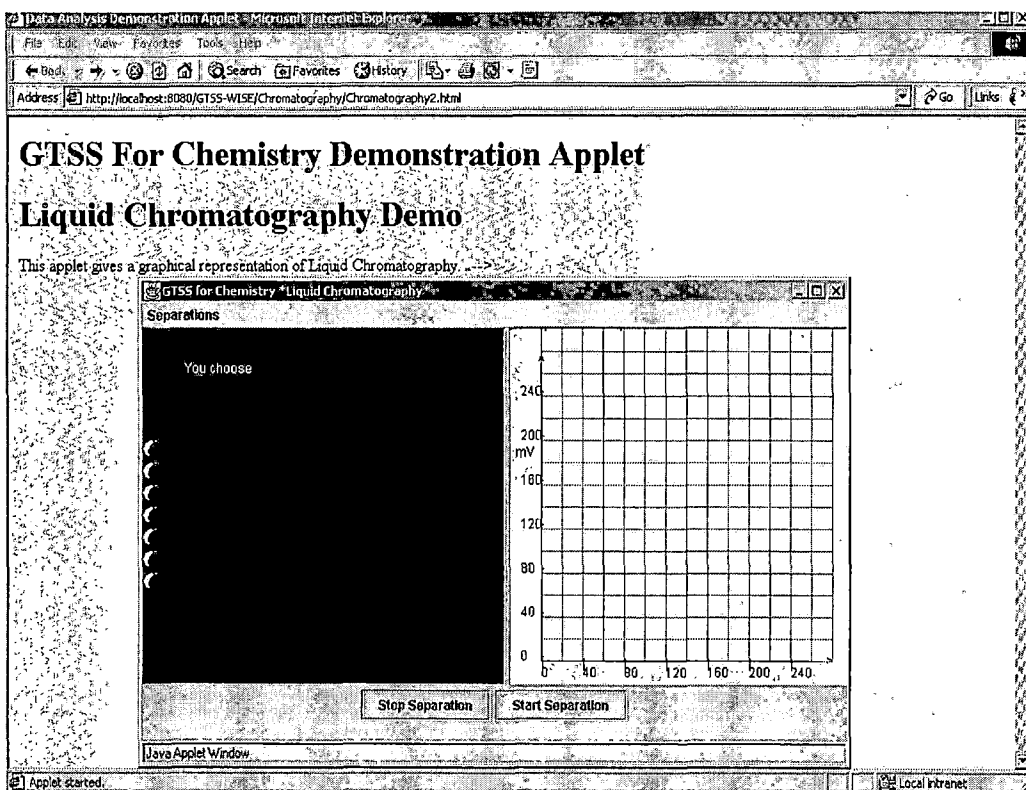


Figure 14. Liquid Chromatography Applet

2.3.1.11 Start New Separation Applet. The Student can start a new liquid chromatography simulation with different parameters (see Figure 15). If the user clicks the mouse button on the "Separations", it will cause a drop-down menu to appear. This will allow the student to choose "New Separation". Each time the result will be different depending on the separation parameters chosen.

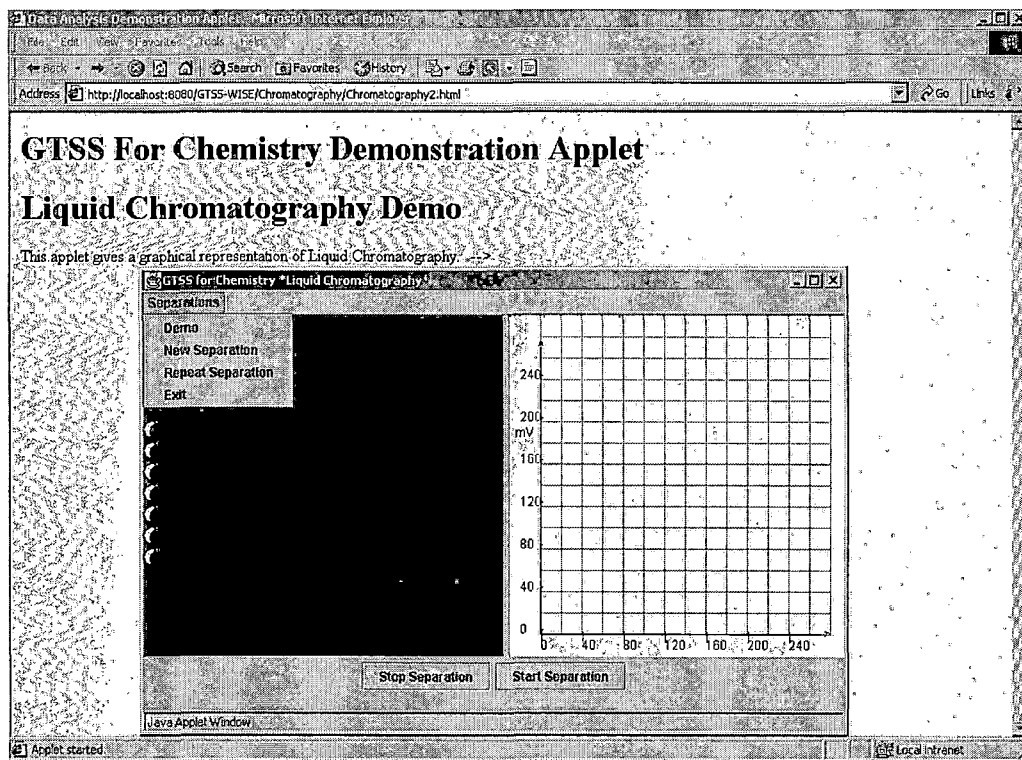


Figure 15. Start New Separation Applet

2.3.1.12 Applet Parameters. Dialog boxes require the student to choose the parameters for the new separation applet. The student will select the numbers of compound to separate. Then he selects the compound name for each component, and the solvent. The student will get an error message if they choose the same compounds (see Figure 16).

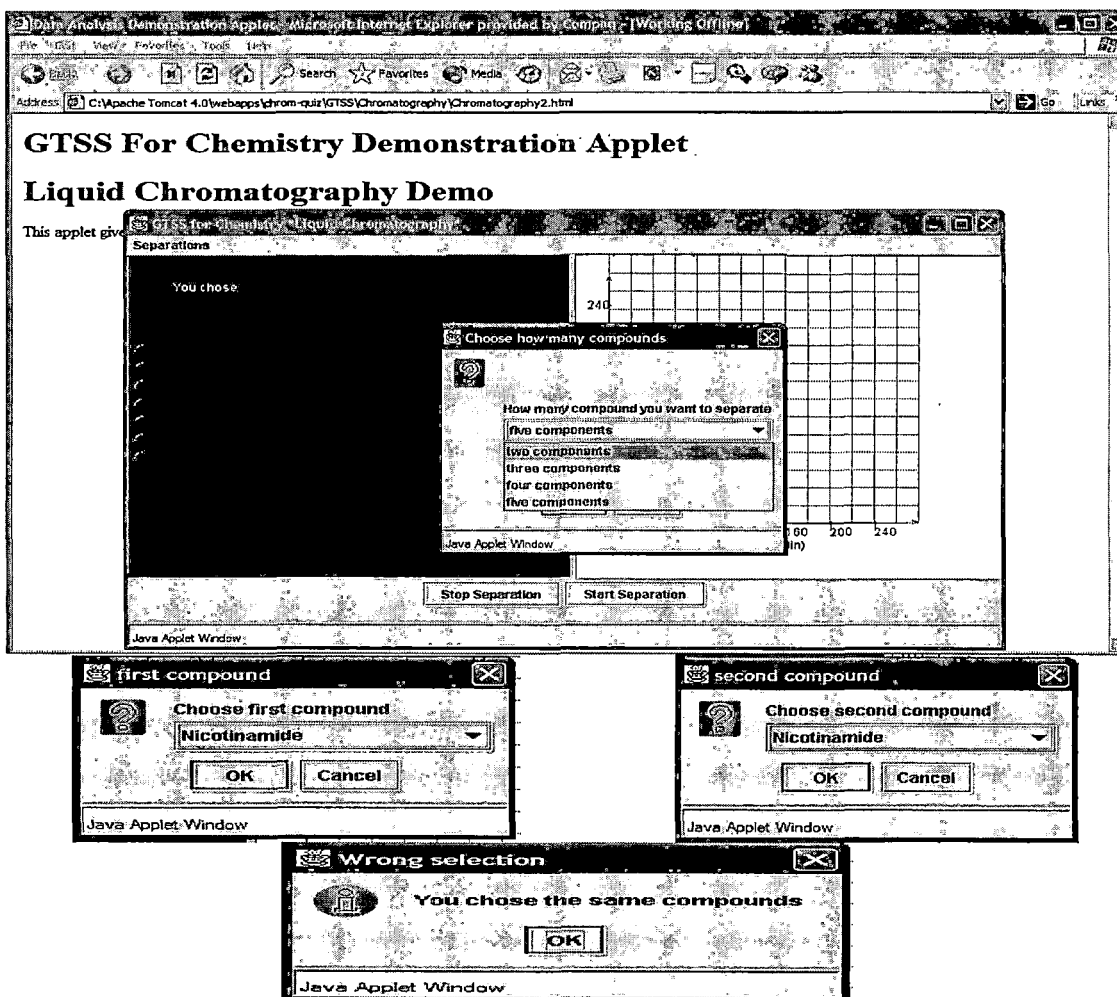


Figure 16. Applet Parameters

2.3.1.13 Separation Report. After the student has selected the parameters, a summary report about the separation conditions appears (see Figure 17). If the student wants to change the parameters, he can click on the "cancel" button and go back to beginning.

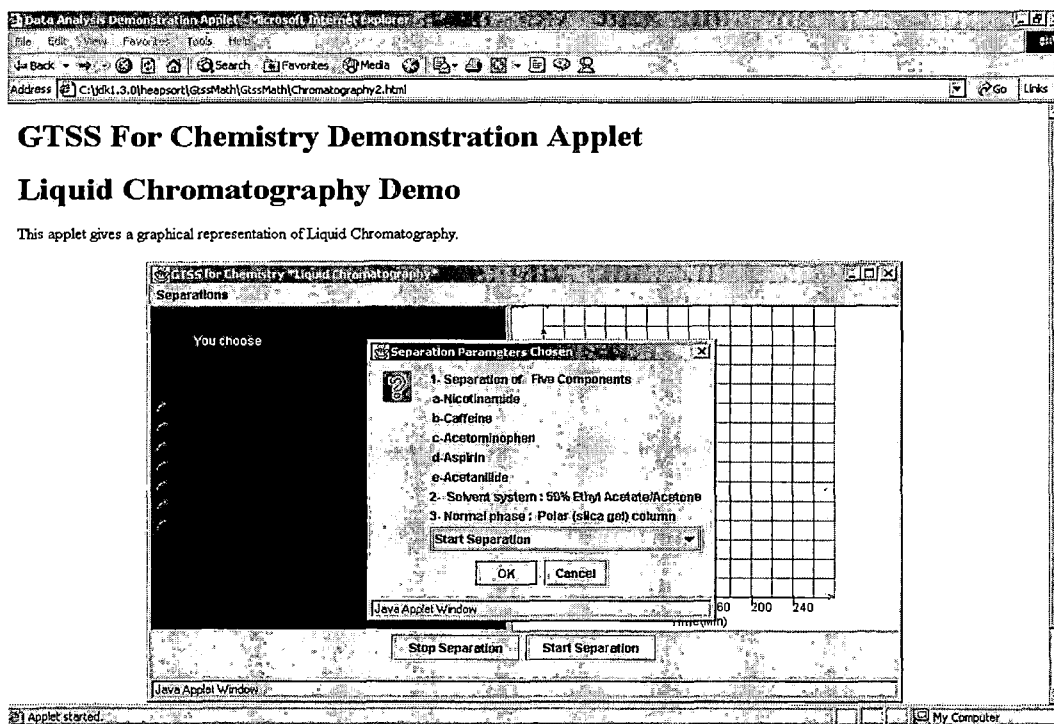


Figure 17. Separation Report

2.3.1.14 Start Separation. After the student confirms his selection and clicks the "Okay" button, the separation applet will start. The components move through the column from left to right, and as they exit the column, a peak is drawn in the x-y plot. Each component is assigned a color and is listed below the column as it. When separation applet is finished, the user will have several options. He can repeat the simulation with the same parameters or he can choose different parameters for a new simulation run.

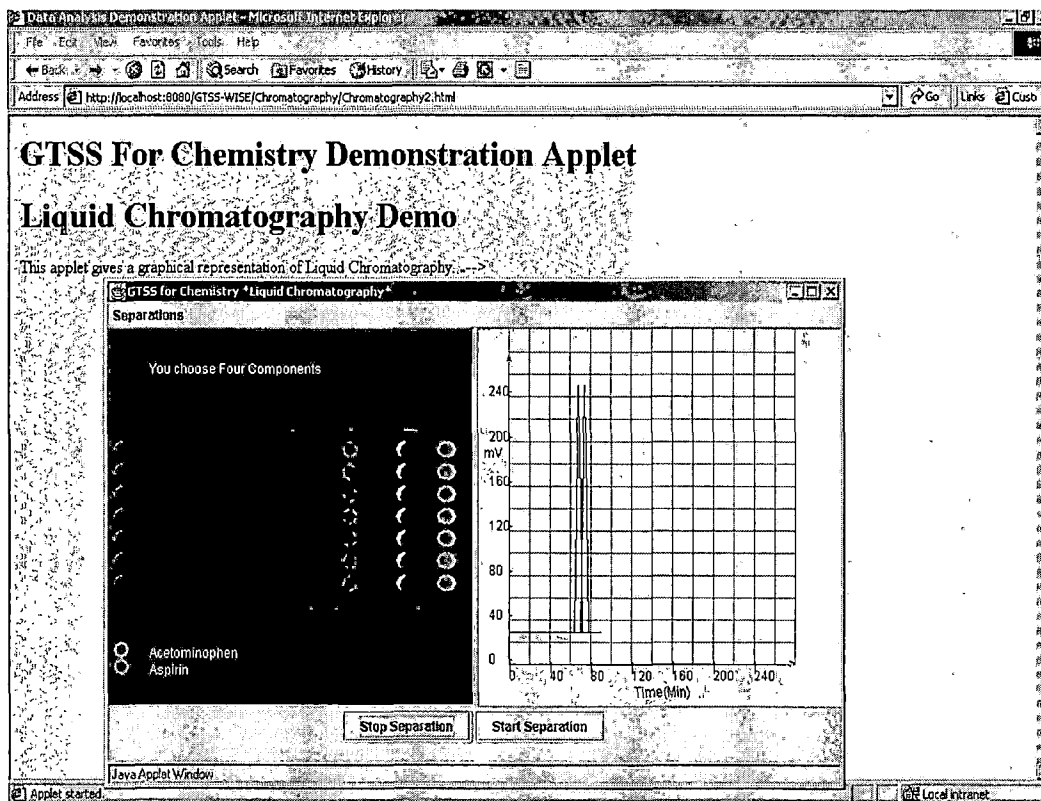


Figure 18. Start Separation

2.3.1.15 Administrator Menu. The welcome page will link to different tasks on Chrom-Quiz system (see Figure 19). "View Instructor-Student information" will allow the administrator to delete or update a student or instructor account. The administrator can also create new accounts for instructors who will use the Chrom-Quiz system.

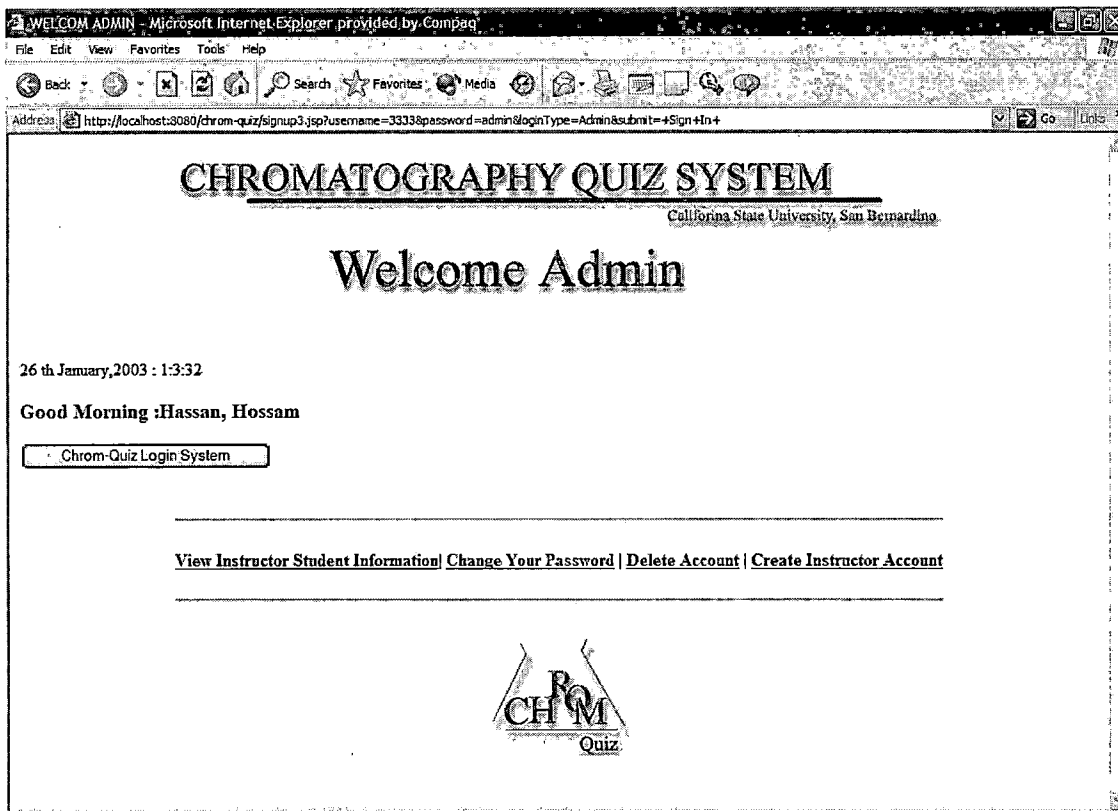


Figure 19. Administrator Menu

2.3.1.16 View Instructor and Student Information

Page. This page allows the admin to access the student and instructor information (see Figure 20). Also, the administrator can delete student accounts to manage the database tables.

Instructors and Student Information - Microsoft Internet Explorer provided by Compaq

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Media Print Mail Stop

Address http://localhost:8080/chrom-quiz/StudentInstructorInfo.jsp Go Links

Welcome To Chrom-Quiz Database System

User Id	First Name	Last Name	E-mail	Login Type	Date Account Created	Update	Delete
5555	hossam	hassan	bhassan84@hotmail.com	Student	2003-01-21 16:06:45	<input type="button" value="Update"/>	<input type="button" value="Delete"/>
User Id	First Name	Last Name	E-mail	Login Type	Date Account Created	Update	Delete
2233	Arturo	concepcion	concep@csci.csusb.edu	Instructor	2003-01-21 20:45:44	<input type="button" value="Update"/>	<input type="button" value="Delete"/>
User Id	First Name	Last Name	E-mail	Login Type	Date Account Created	Update	Delete
1111	Hossam	Hassan	bhassan@csci.csusb.edu	Student	2003-01-21 15:18:21	<input type="button" value="Update"/>	<input type="button" value="Delete"/>
User Id	First Name	Last Name	E-mail	Login Type	Date Account Created	Update	Delete
2222	teacher	chemistry	test200@hotmail.com	Instructor	2002-12-15 22:53:22	<input type="button" value="Update"/>	<input type="button" value="Delete"/>

[View Instructor -student information](#) | [Change Your Password](#) | [Delete Account](#) | [Create Instructor Account](#)

Figure 20. View Instructor-Student Information Page

2.3.1.17 Create New Instructor Account. The administrator can create accounts for instructors who will use the WISE system (see Figure 21). The administrator will fill out the required information to create an instructor account. An instructor account has all the abilities of administrator, except adding and deleting instructors or changing administrator information.

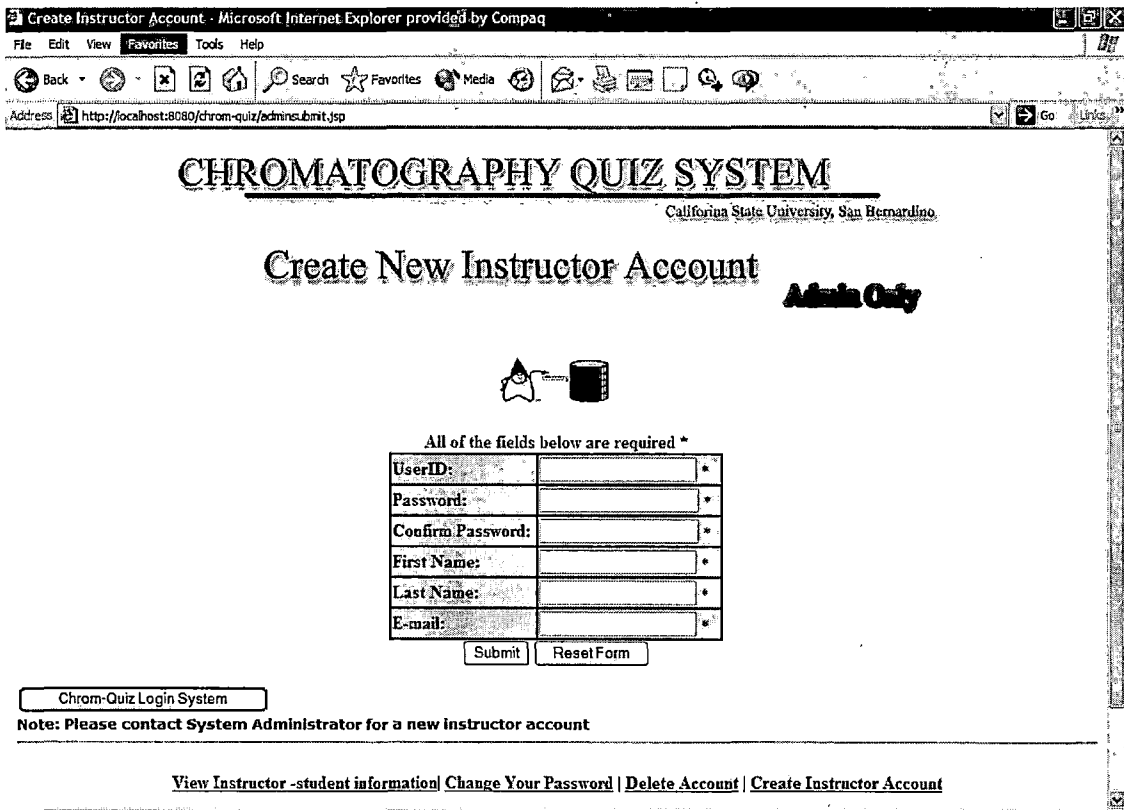


Figure 21. Create New Instructor Account

2.3.1.18 Change Admin Information. This will allow the administrator to change his personal information (see Figure 22).

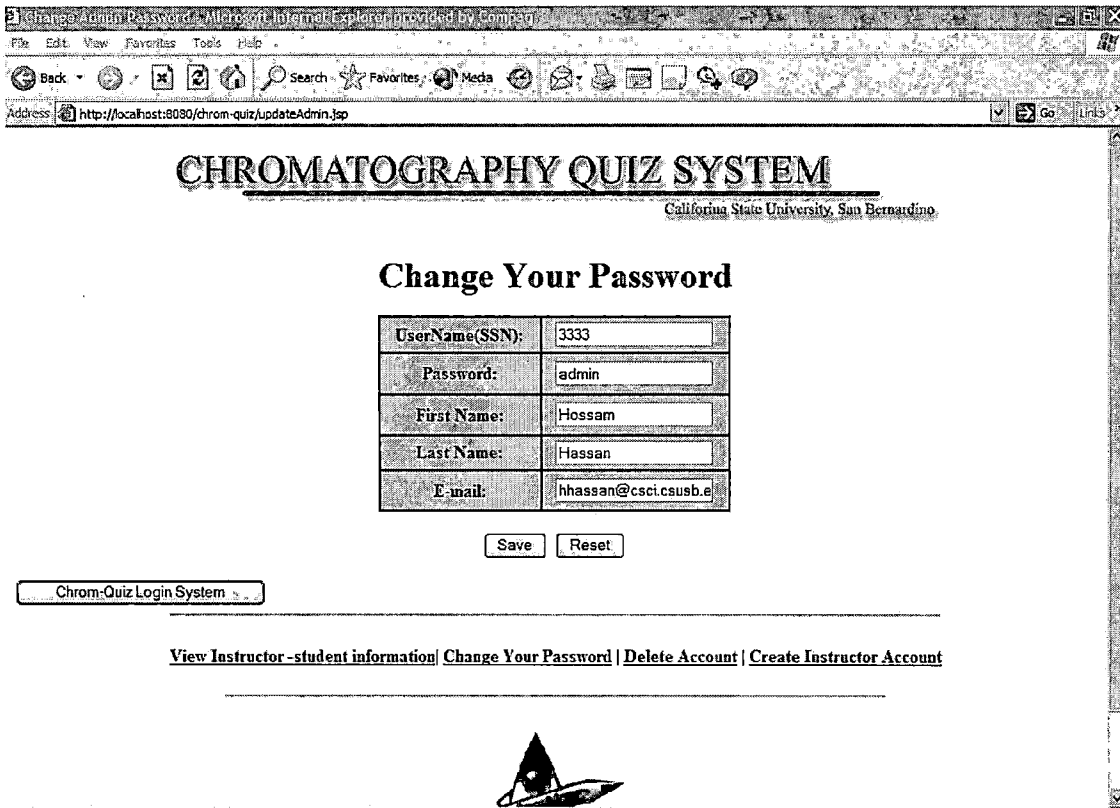


Figure 22. Change Administrator Information

CHAPTER THREE
SOFTWARE DESIGN

3.1 Architecture Design

The software design phase has two parts: architectural design and detailed design. The architectural design and the detailed design describe the product in modules. Unified Modeling Language (UML) is used to analyze the software design of Chrom-quiz system. Most importantly UML explains the complex process of software design in a very simple way. The UML class diagram describes the chromatography engine and how it builds on the top of the GTSS core objects.

3.1.1 Chromatography Engine Design

GTSS project is an on going project in the department of computer science, chemistry, mathematics, and physics at California State University, San Bernardino. Reusing GTSS core objects to create the chromatography engine is one of the most important features of the object-oriented design and is one of the main goals of the GTSS project.

Below are presented the UML class diagram for the chromatography engine, and UML class diagram for the chrom-quiz system.

There are six classes in the core objects that are used to build the new chromatography engine (see Table 2).

Table 2. Core Objects

Class Name	Function
SGApplet	This is the super class of all applet.
SGFrame	Defines a frame.
SGControlPanel	Specifies button on panel.
SGMenu	Specifies menus on menu bar.
SplashPanel	A panel used for demonstration.
VsplitPanel	Defines a two vertically split panels
HspiltPanel	Defines a two horizontally split panels

Chromatography engine consists of three classes: checkersPanel.java, lineGraph.java, and application objects chromatography.java. A unique property of using java language is its support for multithreading (multitasking) that was used for design the chromatography applet animation. The main thread is actually the main program chromatography.java, which is designed to create and start the other thread at the checkersPanel.java. Once initiated by the main thread, the thread starts to run. The thread is implemented in the checkersPanel class, which contains a method called run(). The run() method is

the core of any thread, which is made up of the entire body of any thread. During the lifetime of a thread, it includes many states: newborn state, runnable state, running state and dead state (see Figure 23).

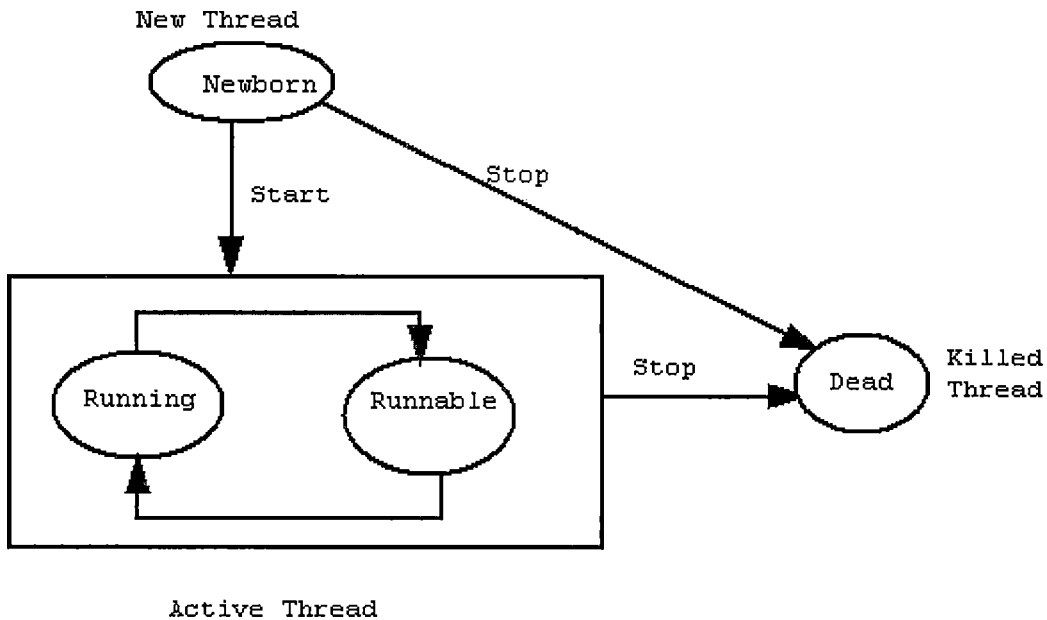


Figure 23. Thread Lifetime Diagram

In the newborn state, the thread is born and is not yet scheduled for running. At this state, it schedules to run using the start() method, or it kills the thread using stop() method. In the runnable state, the thread is ready for execution and is waiting for the availability of the processor. In the running state, the processor has given its time to the thread for its execution. An active thread ends its life when it has completed execution its run()

method. We can call it as a natural death (dead state). On the other hand, we can kill it by sending the stop() method. A thread can be killed as soon it is born or while it is running.

Figure 24 shows the class diagram of the chromatography engine. The class diagram illustrates how the core objects of the GTSS are linked to the Chromatography engine. Also, it shows the relationship between the different classes. The class diagram shows that the chromatography class is the heart of the chromatography engine. There is an aggregation relationship between the lineGraph, checkersPanel and chromatography class, which is shown by a diamond. This relationship identifies how the lineGraph and checkersPanel are parts of the chromatography class. Also, the class diagram shows the dependency or, uses relationship between the chromatography class and the GTSS core classes. The dependency relationship is shown with a dashed line and open arrowhead (see Figure 24).

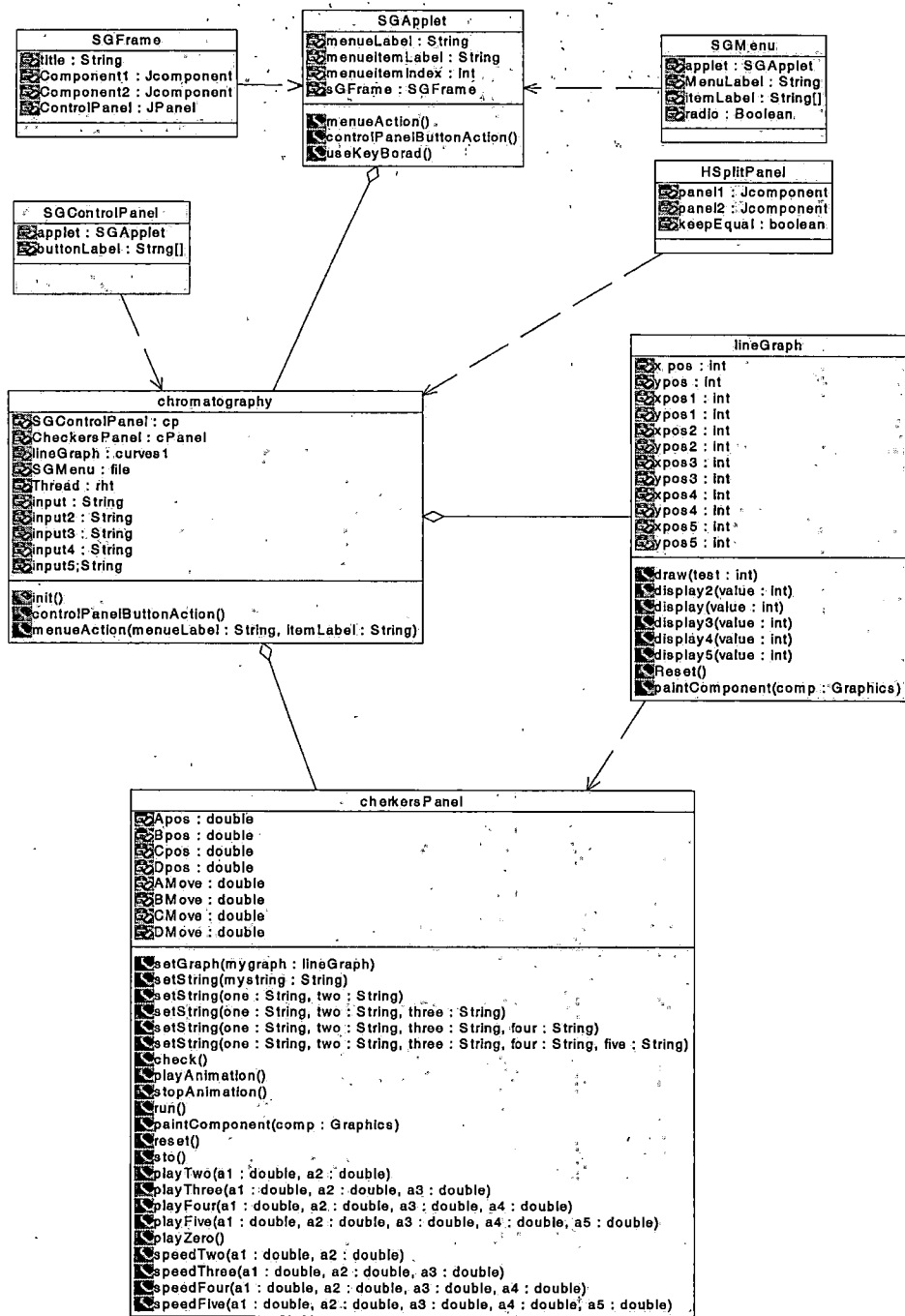


Figure 24. Chromatography Class Diagram

3.1.2 Chrom-Quiz System Design

The Chrom-Quiz system was developed using model view controller (MVC) patterns. MVC is applied to software development to separate the application data from the application code. The Chrom-Quiz system is web application that collects data and stores it in a database. Also, it requires the users to login to the system before accessing any of the pages. The front controller recognizes the source of the request from the clients. The controller determines which view or JSP page to display the current data (see Figure 25).

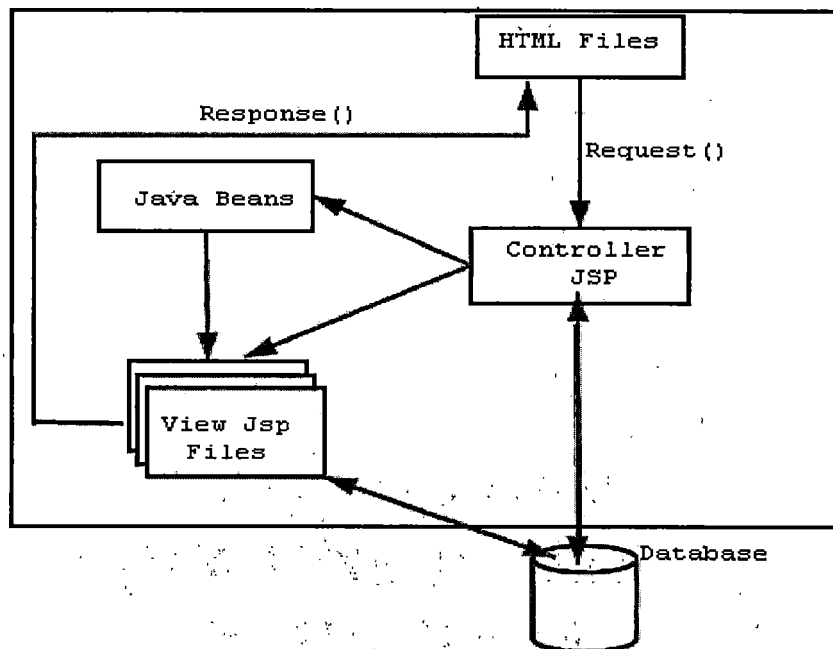


Figure 25. Chrom-Quiz Architecture

Once the specific view has chosen, the JSP makes use of several helpers consisting of either custom tags or JavaBeans. Figure 26 shows the framework of the Chrom-Quiz system and the flow of the web application. The front login controller works as a single point of entry into Chrom-Quiz WEB application (see Figure 26).

The following sequence diagram (Figure 27) shows how the JSP engine supports the compilation of JSP files into a servlet. The servlet handles request from the client and generates a response to the client (see Figure 27).

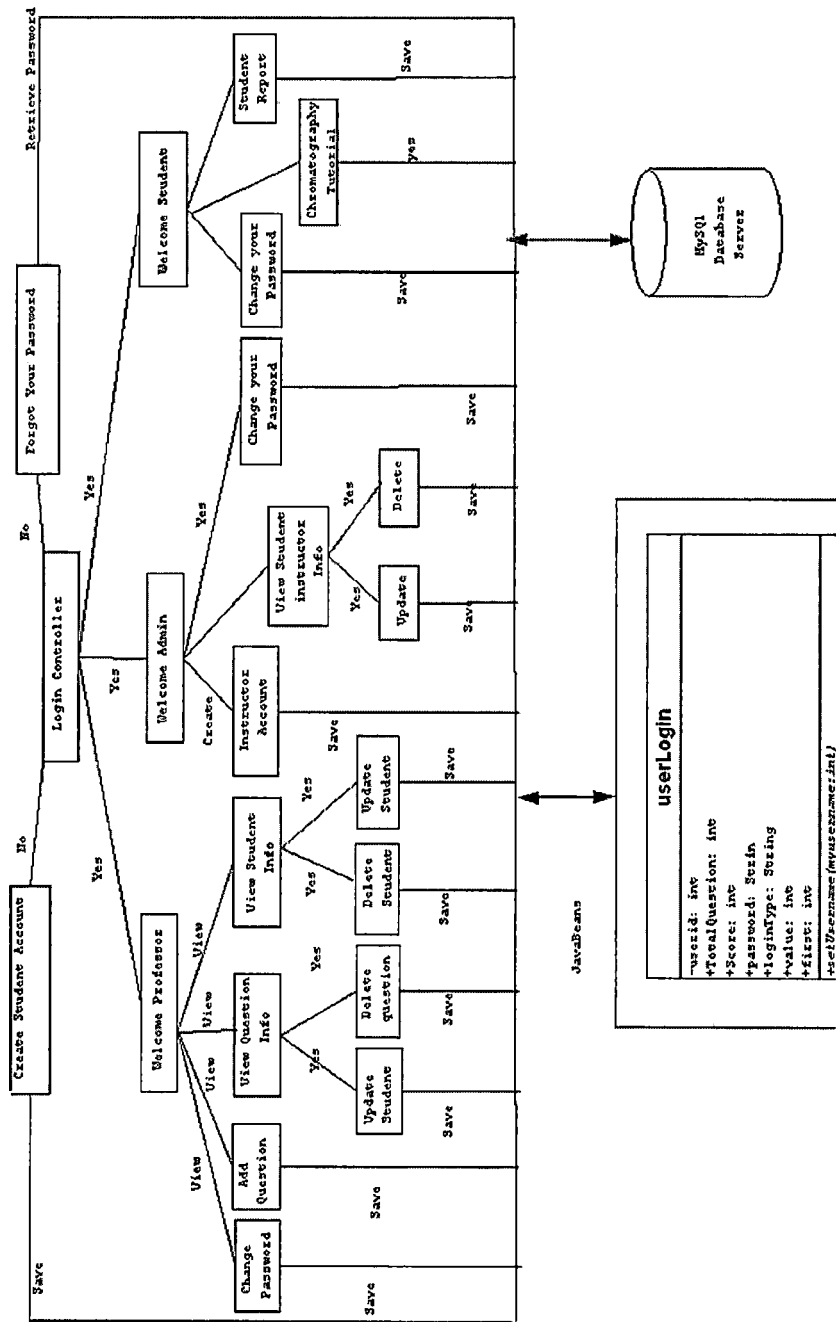


Figure 26. Chrom-Quiz System Frameworks

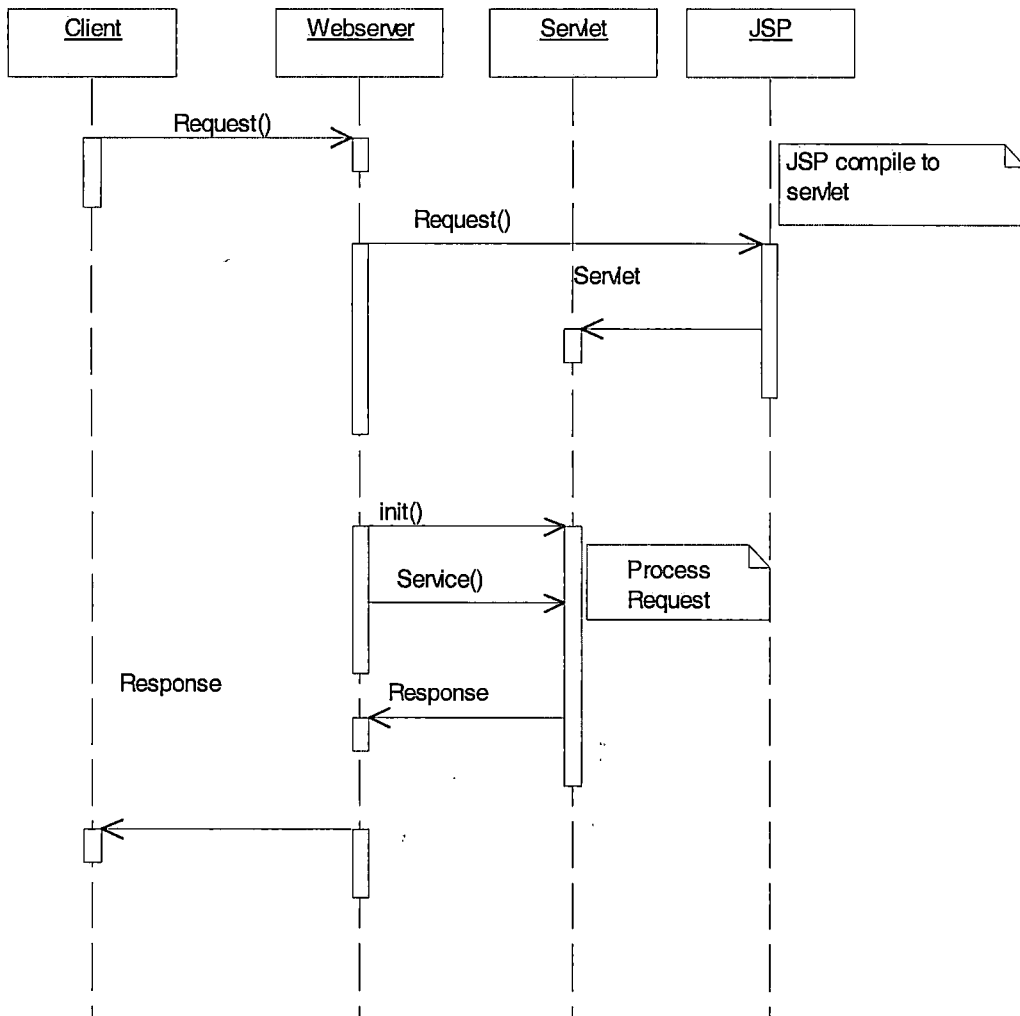


Figure 27. JSP Engine Compilation Diagram

The Chrom-Quiz sequence diagram (see Figure 28) shows how the JSP files exchange information during client request. Validating files plays a very important role as an entry point to secure the Chrom-Quiz system. Validation also controls the direction of the web application.

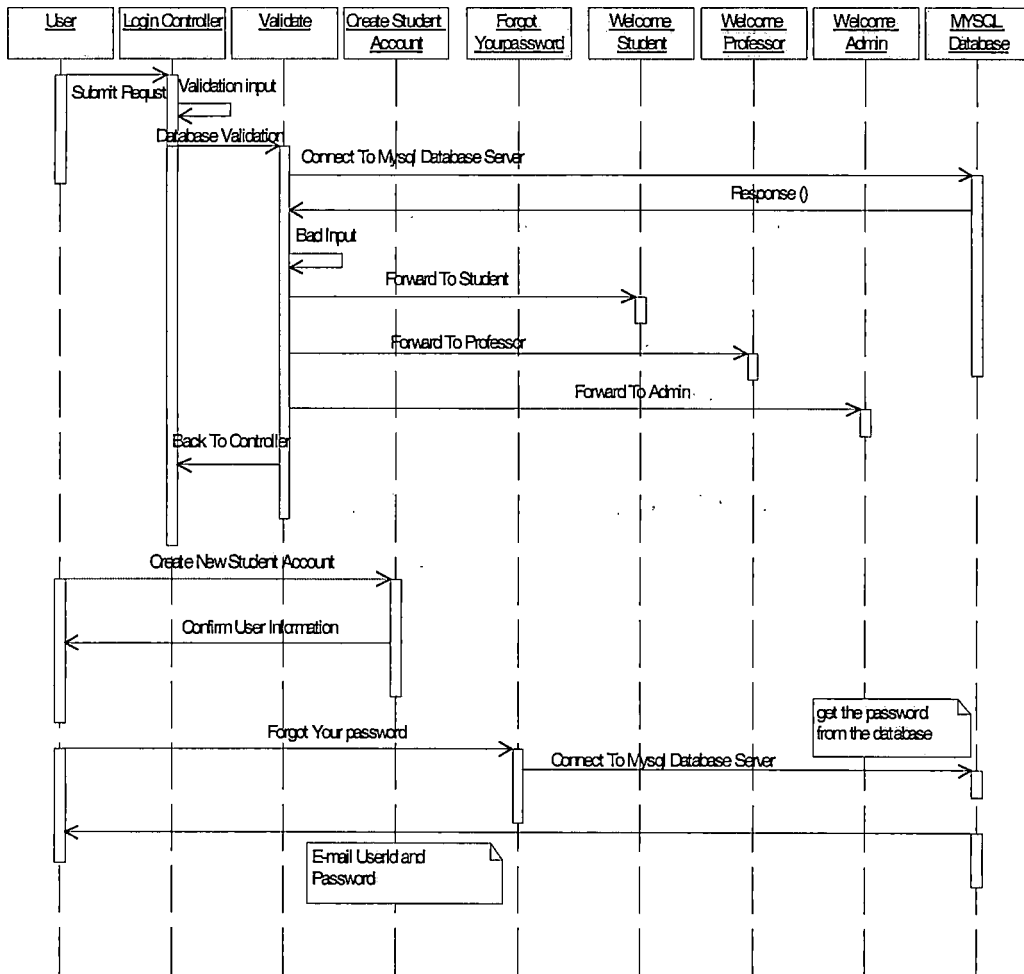


Figure 28. Chrom-Quiz Sequence Diagram

The student sequence diagram (see Figure 29) shows how the JSP files exchange information during a student request. The student JSP file will set up the information about each user. Using Java Beans the user is set up an object. When the student takes the quiz, the student's score will be saved in the database as shown in Figure 29.

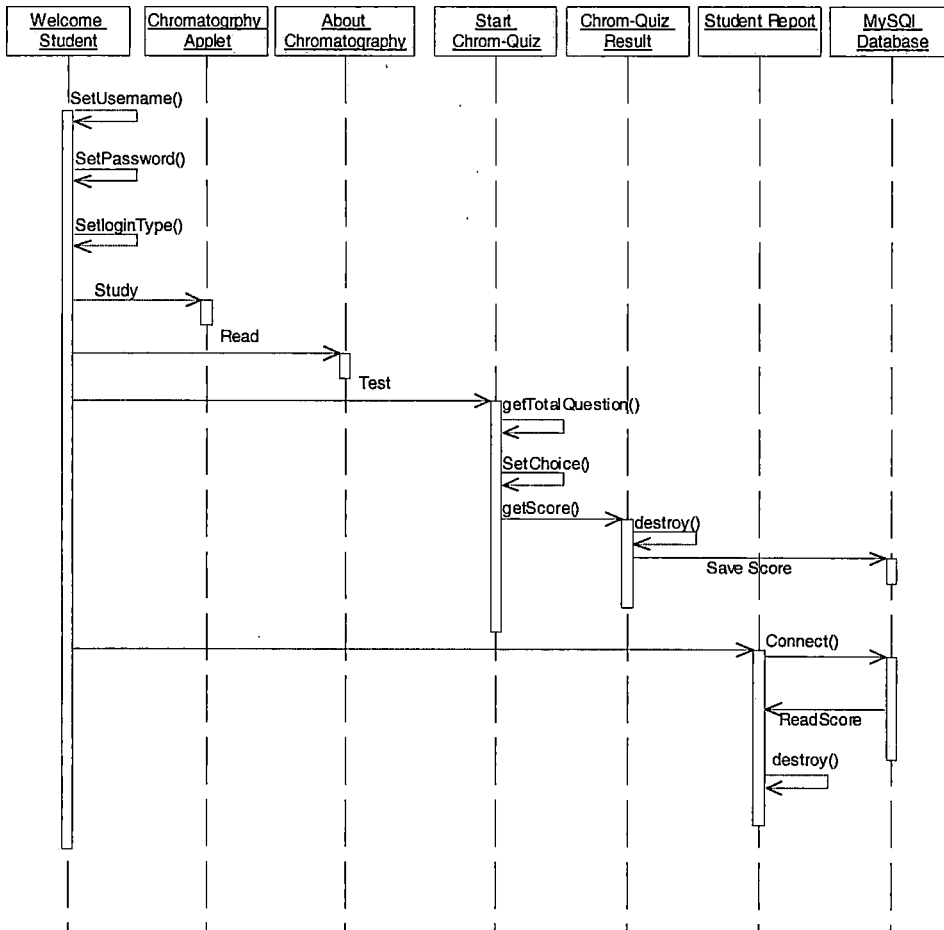


Figure 29. Student Sequence Diagram

The professor sequence diagram shows how the JSP files are exchange information during the instructor's request. The professor can use many features of the Chrom-Quiz system to update information as shown in Figure 30.

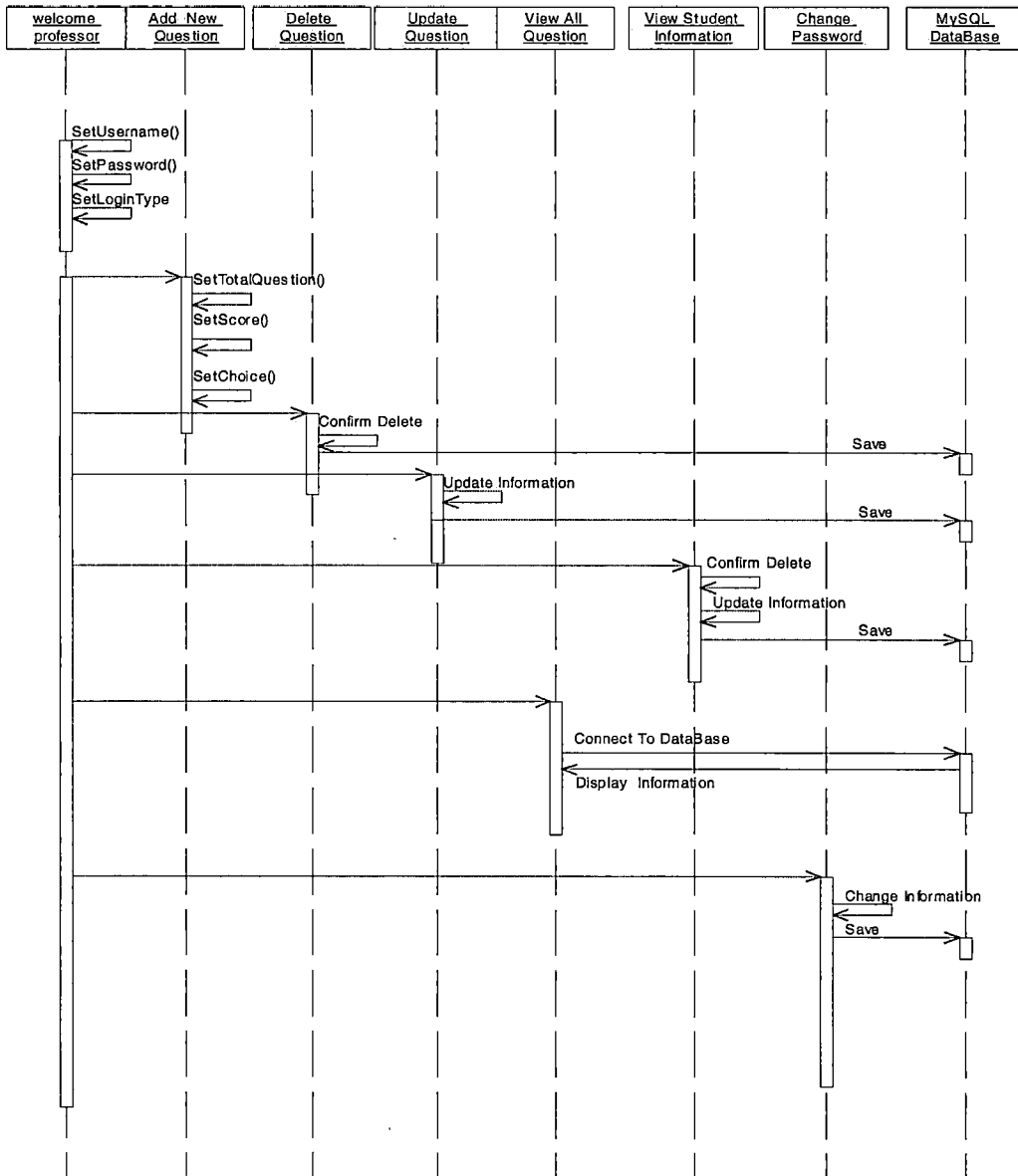


Figure 30. Professor Sequence Diagram

The administrator sequence diagram shows JSP files that will be available for the administrator request. The

administrator can maintain Chrom-Quiz system using many features accessible as shown in Figure 31.

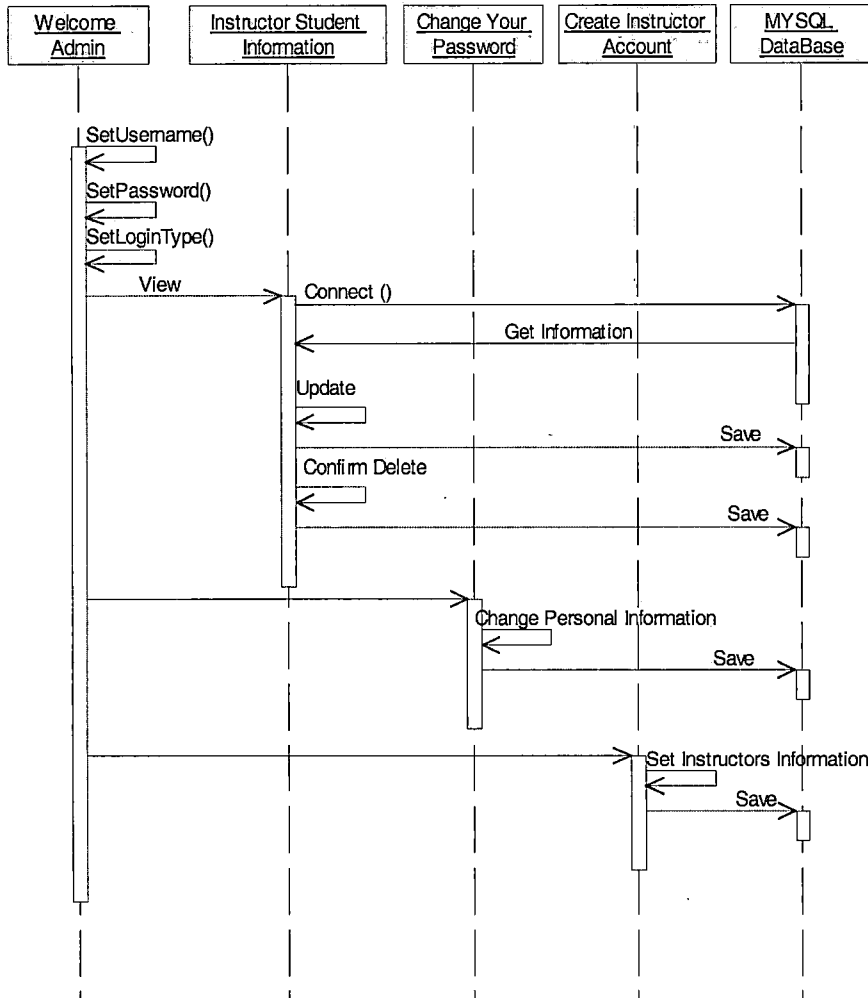


Figure 31. Administrator Sequence Diagram

3.1.3 Database Access Models

The Java application talks directly to the data source require a JDBC driver that can communicate with the particular data source being accessed. Application

commands are delivered to the database, and the results of those statements are sent back to the user (see Figure 32).

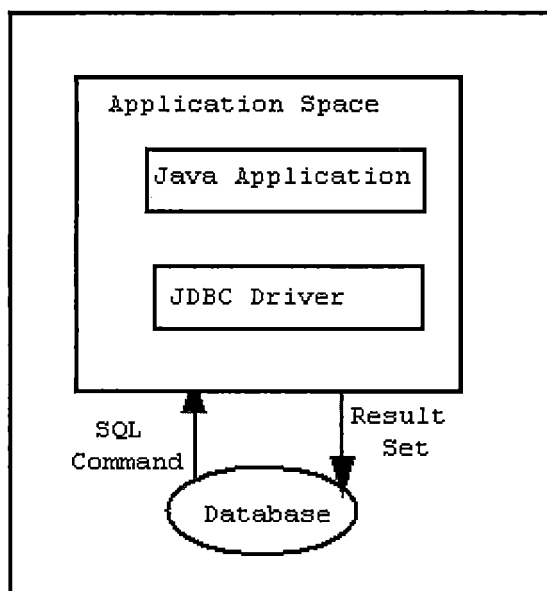


Figure 32. Database Access Models

Figure 33 shows the Chrom-Quiz ER database schema as an ER diagram. Entity types such as User_information, Chromatography_Questions, and Save_Report are shown in rectangle boxes. Relationship types such as study, see, save, and update are shown in diamond shaped boxes attached to the participating entity types with straight lines. Attributes are shown in ovals, and each attributes attached by a straight line to its entity type. Key attributes have their names underlined such as question_id and student_id. ER diagram shows the design of the

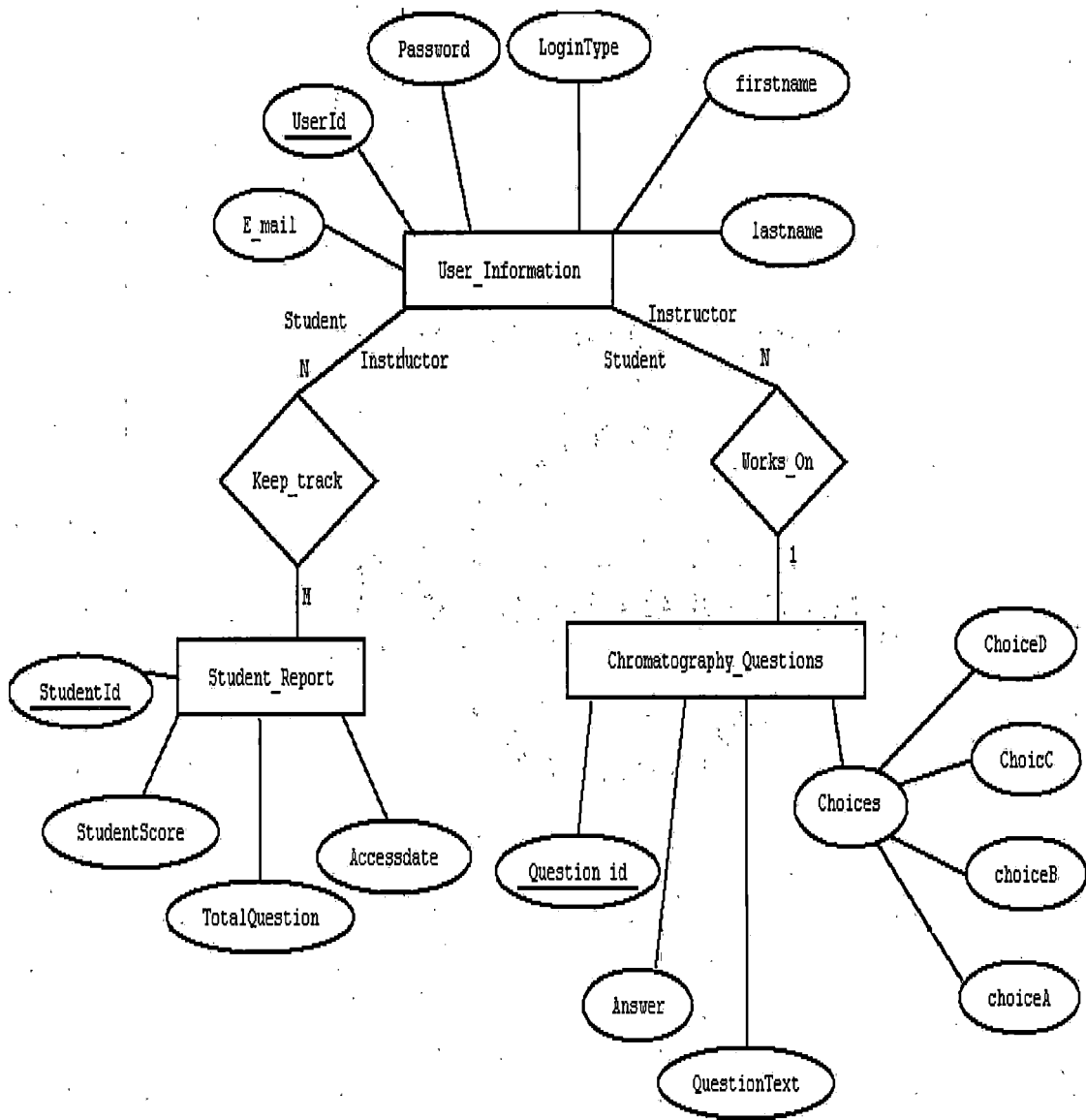


Figure 33. ER Diagram for GTSS/Chrom-Quiz System

Chrom-Quiz database. For example the instructor can work on the chromatography questions. After the instructor

updates the questions, the students start to take chromatography quiz. Student can save their result into the student_report table. Also, the instructor can keep track of the student results. In the ER diagram, the domain of the attribute in any row of the table is a single atomic value. So, the chromatography questions, User information, and student report tables are complied for the first normal form.

Each table is an entity and the field name contains the attributes of this table. Data types of the attributes are depended on the field type. The type of the field could be a string, number, and long text. The following database tables show the detailed entities and attributes for the tables that are used to store the information in the GTSS/Chrom-Quiz web application.

Table 3. User Information

Field Name	Data Type	Description
UserId	Int(11)	User login Id
Password	Varchar(32)	Password for user
Firstname	Varchar(32)	User's first name
Lastname	Varchar(32)	User's last name
Email	Varchar(32)	User's Email
LoginType	Varchar(32)	Student, Instructor, Admin
DateTime	Datetime	Day stamp

Table 4. Chromatography Questions

Field Name	Data Type	Description
QuestionText	Text	Question body entered as a text
ChoiceA	Text	First choice enter as a text
ChoiceB	Text	Second choice enter as a text
ChoiceC	Text	Third choice enter as a text
ChoiceD	Text	Forth choice enter as a text
CurrentDate	Varchar(20)	Current day
CurrentTime	Varchar(20)	Current time
Question_id	Mediumint(9)	This is the primary key
Answer	Varchar(32)	Answer key for the questions

Table 5. Student Report

Field Name	Data Type	Description
StudentId	Int(11)	Student loginId
TotalQuestions	Int(11)	Total question
StudentScore	Int(11)	Student result
Accessdate	Datetime	Current date
Quiznumber	Int(11)	Primary key for Chrom-Quiz

3.2 Detailed Design

Detailed design shows the Java Beans class that is used for the Chrom-Quiz web application. The detailed design will give brief information about Java source code, as comments, bracket `/*. */`.

3.2.1 userLogin Class

```
/*GTSS package for Chrom-Quiz System
GTSS package is a unique name to make a best use of
package. This package stored under directory: C:\Apache
Tomcat 4.0\webapps\chrom-quiz\WEB-INF\classes\GTSS.
*/package GTSS;
//io= input and output
import java.io.*;
Begin userLogin class
public class userLogin{
/* Stores the private data for a user. Every time the
new user access to the GTSS/Chrom-Quiz, an object will
create for this user/
public void setUsername(int myusername){
/* store username to in private data after reading from
the database. Validate that username is matched with the
one that is stored in our database system. If the user
name does not exist on the data base . it will not allow
the user to assess to the Chtom-Quiz System
public void setPassword(String mypassword){
/*save mypassword after accessing the database system
and confirm that this password is matched*/}

public void setLoginType(String myloginType){
```



```

/* assign myloginType to the private data in the
userLogin. There are three login types for accessing the
Chrom-quiz. This method reads from the database and
setups the login type to the private variable in
userLogin class */
}

public void setTotalQuestion(int myTotal){
/* assign myTotal to the private data. This method read
from the database and setup the total questions */

public int getTotalQuestion()
{ /* every time you are calling this method, it returns
the total question in the database*/ }

public int getScore()
{ /*getscore() method return the score of the student and
save it in our database system */}

public void setChoice(int answer)
{ /*This method will store the student answer in an array
The first answer assigns to the first element in the
array and second in the second element until the
student finish all the questions */
questionid[i]= answer;
System.out.println(questionid[i]);
i++; every time you are calling the method the index
will increase one*/}

public int [] getnumber(){
/* This method will return all the user answers as
array. Also this method can access from JSP files. Every
time a new user access to the Chrom-Quiz application,
new sets of answer assign into the array */
}

public void setSore(int myScore){

```

```

/* this method assign student score to the private data.
Once the score is assigned to the private data.we can
access it save in the database */
public int getTotalQuestion()
{
    /* This function is important because every time you
are calling this function, it returns the total question
in the database. Also when the instructors changed the
total question, then we can call this method to setup a
new total question */
}
public int getUserId()
{
    /*
Use this method to iterate through Java server pages and
access the database
*/
}
public String getPassword(){
/*
The password of the student is in the private data in
the userLogin object*/}
public String getLoginType()
{
/* this method will return login type
*/
}

```

Figure 34. User Information Class

CHAPTER FOUR

TESTING

Testing the software product is one of the most important steps in the software life cycle. Testing is the process of running the software product with known testing data to find errors on the output data. Most importantly testing is necessary to ensure the utility, reliability, robustness, and performance of the software product.

4.1 Testing Plan

The testing plan for Chrom-Quiz system consists of unit testing, integration testing and system testing. Starting with the unit testing is efficient way to detect any errors in the application when building process of the Chrom-Quiz System.

4.2 Unit Testing

Unit testing is a process for the validation of a small part from a complex software system. By using unit testing, defects of the Chrom-Quiz system can be detected and removed. The unit testing can be divided into three parts: functional testing, structural testing, and intuitive testing. Functional testing helps to find any wrong implementations in the Chrom-Quiz System. Structural

testing helps to find anything unexpected and any wrong implementations. Intuitive testing helps to catch any errors on the system. Unit testing results of the Chrom-Quiz are shown in Table 6.

Table 6. Chrom-Quiz Unit Testing

Forms	Test performed	Result
Login Page	<ul style="list-style-type: none"> • Check submit and Reset buttons • Ensure all links works • Verify the validation of the input date. 	Pass
Authorization	<ul style="list-style-type: none"> • Verify only the correct data can gain access to Chrom-Quiz system and forward to the correct Web page 	Pass
Create New student Account	<ul style="list-style-type: none"> • Check submit and Reset buttons • Ensure all links are working as expected. • Verify the validation of the input text to create a new student account. • Ensure all the input questions texts save in the database. 	Pass
Forget Your Password Page	<ul style="list-style-type: none"> • Verify the E-mail address. • Verify the e-mail's sent to the client. 	Pass
Student Main Menu	<ul style="list-style-type: none"> • Verify the validation of the student name. • Test to make sure that button and links are correct. • Verify that the Chrom-Quiz test and automated score system are working properly. 	Pass

Forms	Test performed	Result
Tutorial Chrom-Quiz	<ul style="list-style-type: none"> • Ensure the button and links are working as we expected. • Test window navigation using the mouse and keyboard. 	Pass
Liquid Chromatography Applet	<ul style="list-style-type: none"> • Make sure that the applet is running with the Explorer and Netscape browsers. • Ensure that all drop-down menus buttons, and boxes properly working as expected. • Make sure that the selection of the compounds works as expected and give the correct results. 	Pass
Student Score Page	<ul style="list-style-type: none"> • Make sure every time a student takes the Chrom-Quiz, results are saved in the database. • Ensure that all buttons and links are working. 	Pass
Instructor Main Menu	<ul style="list-style-type: none"> • Verify the validation of the instructor name. • Ensure that button and links are working. 	Pass
Add New Question	<ul style="list-style-type: none"> • Check submit and Reset buttons • Ensure all links are working as expected. • Verify the validation of the input text to create a new question. • Ensure that the input text is save in the database. 	Pass
Change Password	<ul style="list-style-type: none"> • Check submit and Reset buttons • Make sure the instructor can change his personal information on the database. • Ensure all links are working as expected. 	Pass

Forms	Test performed	Result
View Student Information	<ul style="list-style-type: none"> • Ensure that update and delete account buttons are working. • Make sure the instructor can update or delete account from the database without access to the user password. 	Pass
Update Questions	<ul style="list-style-type: none"> • Make sure that the instructor is retrieving the question text from the database. • Ensure that the updating question is saved into the database. 	Pass
System Administrator Main Menu	<ul style="list-style-type: none"> • Verify the validation of the administrator name. • Ensure that button and links are working as expected. 	Pass
Change Admin Password	<ul style="list-style-type: none"> • Check submit and Reset buttons • Make sure the admin can change his old password and save the new password on the database. 	Pass
View Student Instructors Account	<ul style="list-style-type: none"> • Ensure update and delete account buttons are working. • Make sure that the administrator can delete student and instructor accounts from the database without access to their password. • Ensure that the updated account is saved into the database. 	Pass
Create New Instructor Account	<ul style="list-style-type: none"> • Check submit and Reset buttons • Ensure all links are working as expected. • Verify the validation of the input text to create a new instructor account. • Ensure that all the input texts are save in the database. 	

4.3 Integration Testing

The integration test is validating that the entire Chrom-Quiz web application works as a one unit as expected. During the integration testing, we can detect any unexpected results of the Chrom-Quiz application while the software product is under development. Thus, it will be easy for the developer to fix before the end of the software lifecycle. Integration testing results of the Chrom-Quiz are shown in Table 7.

Table 7. Integration Testing Results

Integr. Test	Test Performed	Result
Chrom-Quiz tutorial system	<ul style="list-style-type: none">• Test all tutorials and applets• Test chromatography applet parameter as one unit	Pass
Chrom-Quiz users testing	<ul style="list-style-type: none">• Verify the validation of all account data with the database existing on the Chrom-Quiz system.• Validate the creation, modification, and deletion of data in tables as specified in the functionality.	Pass

4.4 System Testing

System testing is necessary for the implementation of the Chrom-Quiz system. It will ensure the Chrom-Quiz reliability and integrity. Testing the Chrom-Quiz involves database testing, user acceptance testing, server load and

security testing. System testing results of the Chrom-Quiz are shown in Table 8.

Table 8. System Testing Results

System Testing	Results
<ul style="list-style-type: none">• Install Chrom-Quiz system into computer science server.	Pass
<ul style="list-style-type: none">• Start up all services on our server such as tomcat 4.0, MySQL server, and zone alarm as security system.	Pass
<ul style="list-style-type: none">• Rigorous testing of Chrom-Quiz system with real data to ensure the reliability and integrity of the system.	Pass

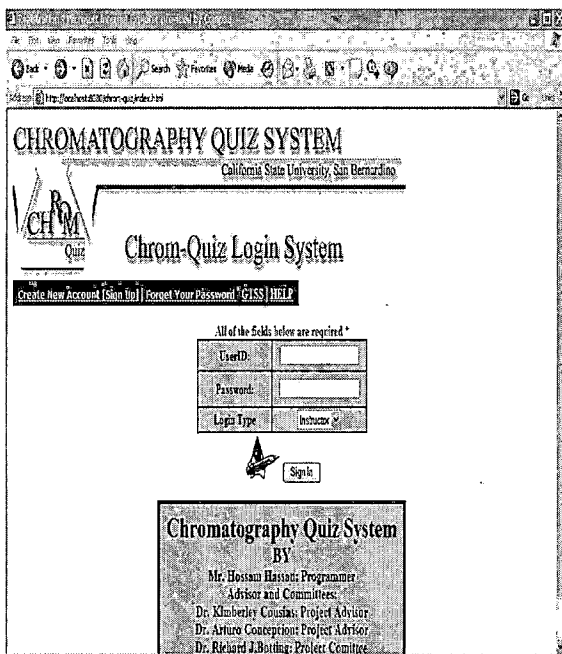
4.5 Complete Testing Scenario

The following section shows a complete tutorial on how to use the GTSS/Chrom-Quiz. Also, it shows an example how the student can view the applet and take the quiz, and how the instructor builds a quiz and manages the GTSS/Chrom-Quiz.

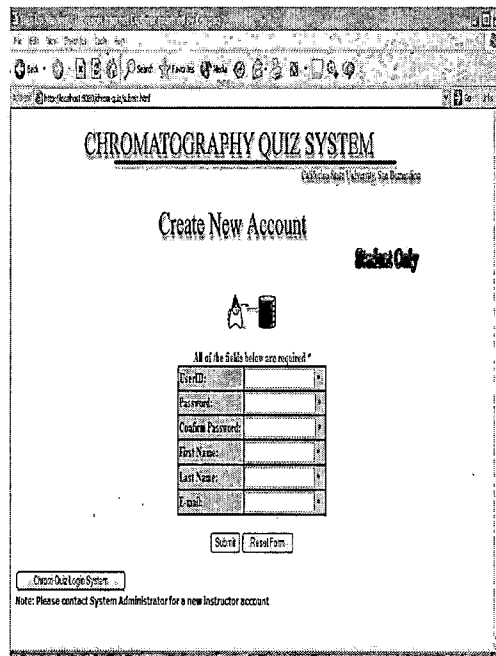
4.5.1 GTSS/Chrom-Quiz Tutorial

This section explains how the users can access the GTSS/Chrom-Quiz web application. The tutorial consists of three pages for using the GTSS/Chrom-Quiz application. The login page for GTSS/Chrom-Quiz System is shown in Figure 35.1. Users have to type the userID, password, and select

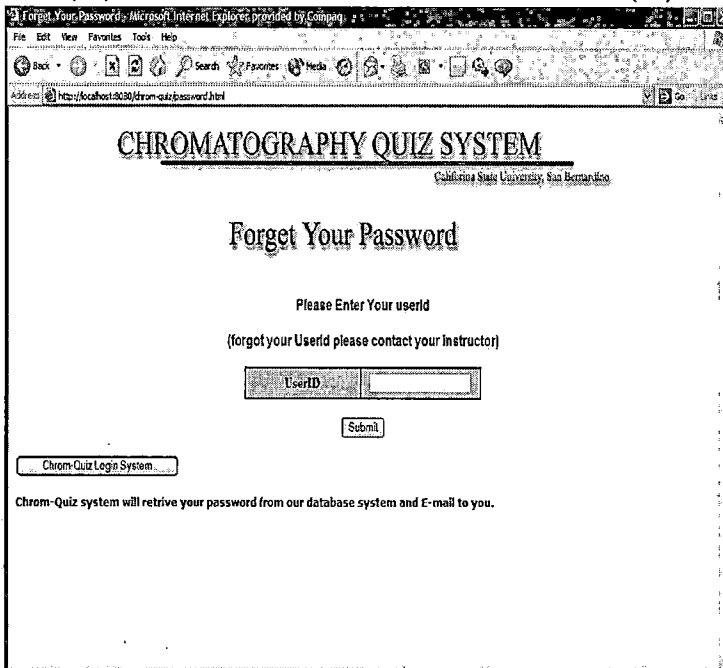
the login type (Student, Instructor, Or Admin). This page works as a entry point to the GTSS/Chrom-Quiz application. Create new student account page will be used for the students who are using the Chrom-Quiz system for the first time (see Figure 35.2). After they fill out the required information, they can access the Chrom-Quiz system. Forget password page will be used for users who forget their password (see Figure 35.3). Users will fill out the required information and click on submit. The Chrom-Quiz system will send their password by e-mail.



(1)



(2)

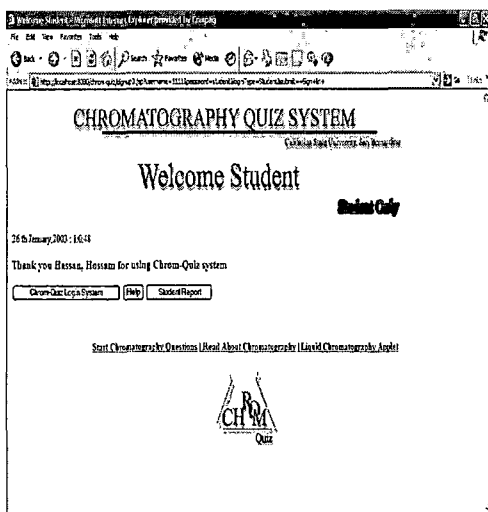


(3)

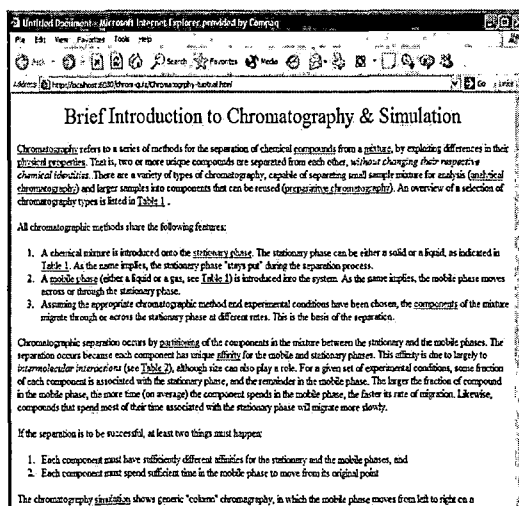
Figure 35. GTSS/Chrom-Quiz Tutorials

4.5.2 Student Tutorial

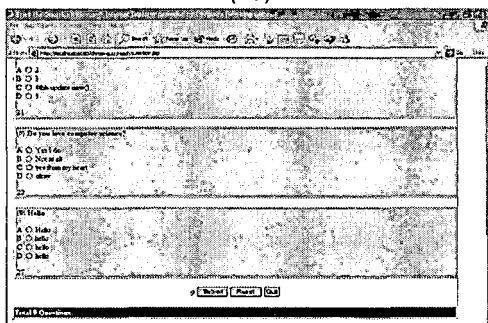
This section consists of two parts. First, the student interacts with the chromatography simulation applet. Second, The student will take the quiz and submit their answer. If the student enters the correct userId and password, he will be forwarded to the student welcome page. The student welcome page will link to different tasks on Chrom-Quiz system (see Figure 36.1). The "Read about Chromatography" button will give a tutorial about the liquid chromatography technique (see Figure 36.2). If the student clicks on "Start Chromatography Questions" button, the exercise questions and Chromatography simulation applet will appear on two different screens (see Figure 36.3). After the student finishes answering the questions and clicks on the submit button, he will get the score of the quiz. The student will have a choice to save this score in the Chrom-Quiz database or go back and repeat the quiz as many times as he want (see Figure 36.4). Also, the student can see his pervious quiz result by clicking the student report link. If the student saves his score in the Chrom-Quiz database, he cannot delete it from the Chrom-Quiz system. The instructor can delete the student scores to manage the database without going to the administrator level.



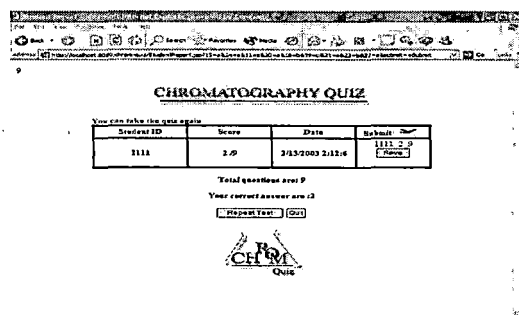
(1)



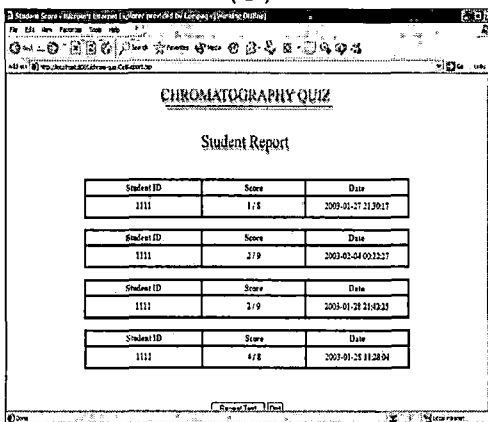
(2)



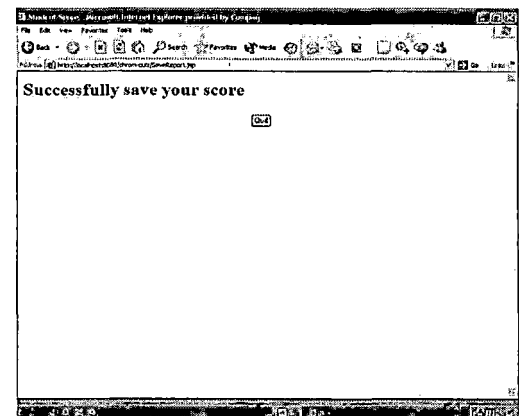
(3)



(4)



(5)

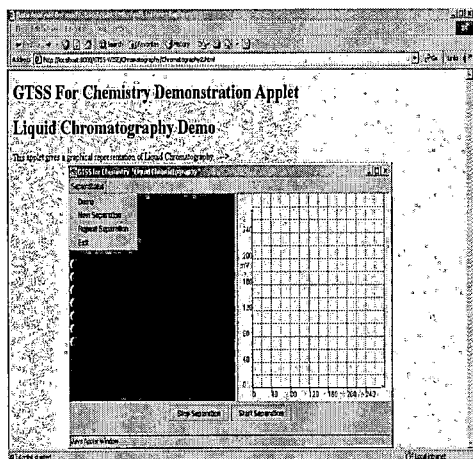


(6)

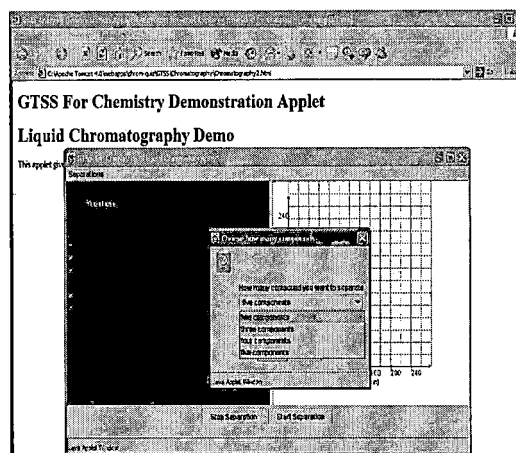
Figure 36. Student GTSS/Chrom-Quiz Tutorials

When the student clicks on "Start Chromatography Question", the GTSS for liquid chromatography simulation will appear in a new window. The student can start a new

liquid chromatography simulation with different parameters. If the user clicks the mouse button on the "Separations", it will cause a drop down menu to appear (see Figure 37.1). This will allow the student to choose "New Separation". The student will select the numbers of compound to separate (see Figure 37.2). He then selects the compound name for each component, and solvent. The student will get an error message if he chooses the same compounds (see Figure 37.3, 37.4, 37.5). After the student has selected the parameters, he will get a summary report about the separation conditions appears (see Figure 37.6). If the student wants to change the chosen parameters, he can click on the "cancel" button and go back to beginning. After the student confirms his selection and clicks the "Okay" button, the separation applet will start. When separation applet is finished, the user will have several options. He can repeat the simulation with the same parameters or he can choose different parameters for a new simulation run (see Figure 37.7).



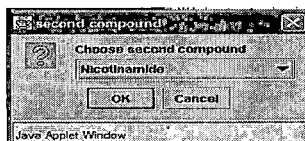
(1)



(2)



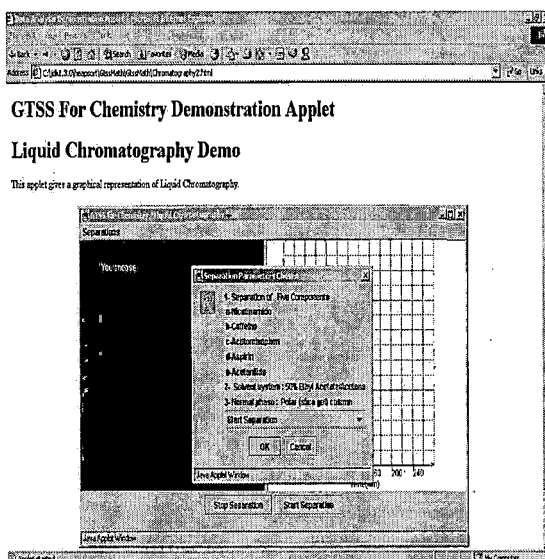
(3)



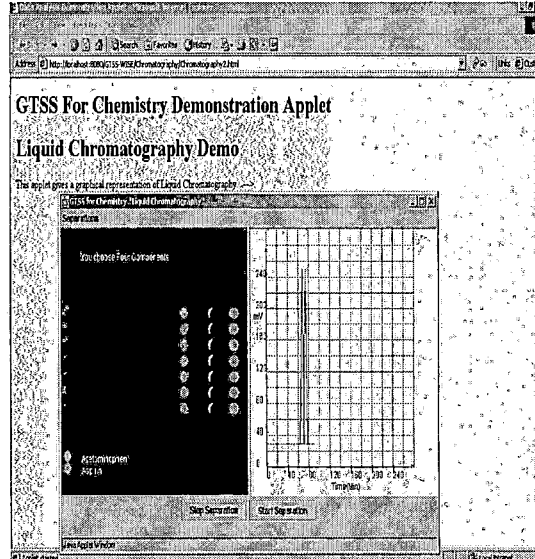
(4)



(5)



(6)



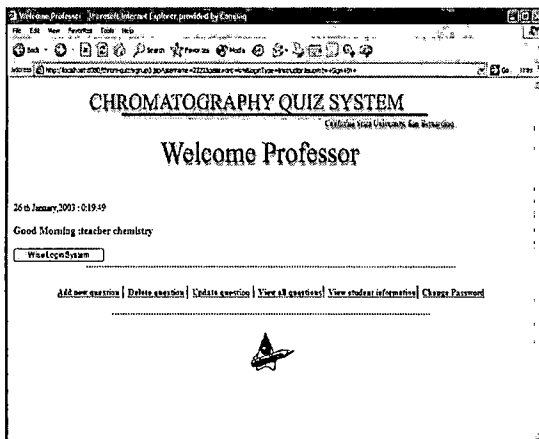
(7)

Figure 37. Chromatography Applet Tutorials

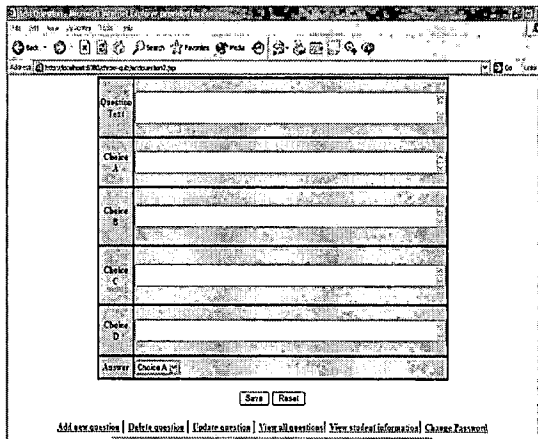
4.5.3 Instructor Tutorial

The instructor welcome page links to different tasks on Chrom-Quiz system (see Figure 38.1). "Add New Question" will allow the instructor to create a new question and

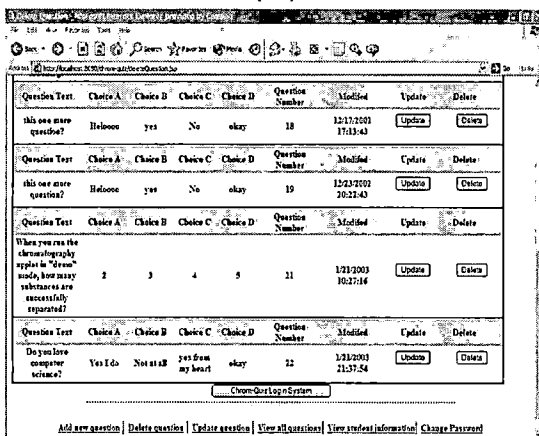
save it on GTSS/Chrom-Quiz database (see Figure 38.2). The Instructor will fill out all of the required information and click on the "submit" button. The GTSS/Chrom-Quiz system will add the information into the database. "Delete question" and "update question" links will let the instructor change the existing questions on in the Chrom-Quiz database (see Figure 38.3). The instructor can access the student information through "View student information" link. The instructor can delete a student account to manage the database without going to the administrator level. In addition, the instructor can view student scores on the Chrom-Quiz (see Figure 38.3). Finally, the instructor can change his/her password by using the "Change Password" link.



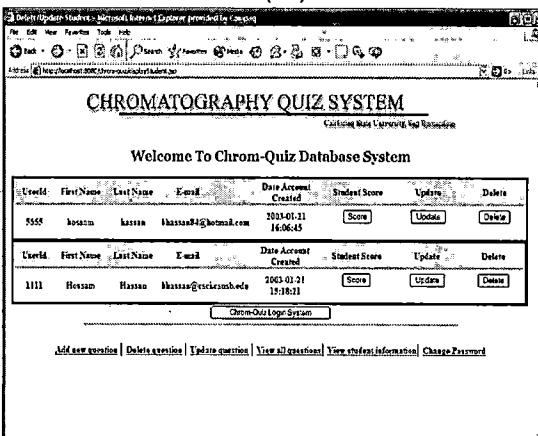
(1)



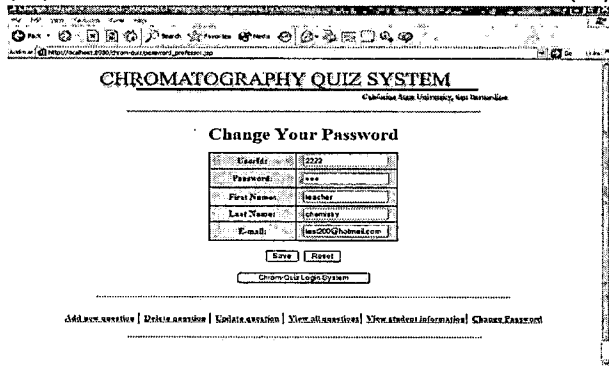
(2)



(3)



(4)



(5)

Figure 38. Instructor GTSS/Chrom-Quiz Tutorials

CHAPTER FIVE
MAINTENANCE MANUAL

Ensuring maintainability is necessarily during the entire software process. The maintenance manual will give clear information about how to maintain the Chrom-Quiz system. There are four levels of maintenance for Chrom-Quiz system: chromatography applet maintenance, Chrom-Quiz Web application maintenance, Web server maintenance and installation, and Mysql Database Server.

5.1 Chromatography Applet Maintenance

There are three java classes in the chromatography engine. To maintain the chromatography engine, the administrator needs experience with Java programming language. Three classes are used to maintain or modify java code. Java classes are locating in edu\csusb\gtss\chem\ directory inside the GTSS package. Java files are shown in Table 9.

Table 9. Chromatography Engine

JAVA classes under Chem Directory
• CheckersPanel.class
• Chromatography.class
• lineGraph.class

Following updating or modifying the Java classes of Chromatography engine, the code must be recompiled and tested as a one unit. All Java classes are under "edu\csusb\gtss\chem\" directory.

5.2 Chrom-Quiz WEB Application Maintenance

There are three levels of maintenance: student JSP files, instructors JSP files, and administrator JSP files. To maintain JSP files, one needs experience with Java server pages and Java programming language. All JSP files are under the apache_Tomcat_4.0\webapps\chrom-quiz directory. Student JSP files are shown in Table 10. Instructor JSP files are shown in Table 11.

Table 10. Student Java Server Pages (JSP) Files

JSP classes under Webapps\ chrom-quiz directory
• WelcomeStudent.jsp
• readyquestion.jsp
• studentReport.jsp
• GetReport.jsp
• Read_About_Chromatography
• liquidChromatography.html

Table 11. Instructor JSP files

JSP classes under Webapps\ chrom-quiz directory
• Welcome_professor.jsp
• addquestion.jsp
• deleteQuestion.jsp
• update.jsp
• displaystudent.jsp
• password_professor.jsp
• UpdateStudent.jsp
• displayQuestion.jsp

Administrator JSP files are shown in Table 12.

Table 12. Administrator JSP files

JSP classes under Webapps\ chrom-quiz directory
• Welcome_admin.jsp
• adminsubmit.jsp
• StudentInstructorInfo.jsp
• updateAdminStudent.jsp
• updateAdmin.jsp
• UdateStudent.jsp

5.3 Install Tomcat Server

The Chrom-Quiz web application is running on the Windows 2000 operating system. The tomcat web server was obtained from the Apache-Jakarta project (<http://jakarta.apache.org>). Tomcat server is an open source servlet container. To add an application to the server, you must create a directory structure underneath the \webapps directory:

c:\tomcat4\webapps\Chrom-Quiz\WEB-INF\lib. Also in the c:\tomcat4\conf\server.xml file, add the following context entry was added:

```
<context path="Chrom-Quiz"
DocBase="Webapps/Chrom-Quiz"
CrossContext="true" Debug="0" reloadable="true"
Trusted="false"> </context>.
```

JSP files can be accessed by entering

<http://localhost:8080/Chrom-Quiz> in the browser Window.

Before starting Java and Tomcat 4 must be configured. In Windows 2000, select

setting/controlPanel/System/Advanced and click Environment

Variables: CATALINA_HOME:c:\Tomcat, JAVA_HOME:c:\jdk1.3.1

and ClassPath :Set Calsspath =

c:\tomcat\common\lib\servlet.jar;c:\tomcat\lib;

c:\tomcat\server\lib; c:\tomcat\common\lib;

5.4 Java DataBase Connectivity and Mysql Database Server

You can download Mysql database server from <http://www.mysql.com>. MySQL database is located at `c:/mysql`. To access the tables in the database server, you need to access to the `c:/mysql/bin/mysql` and you should have some experience with structure quarry language (SQL). JDBC is located at `c:/jdbc`. In order to use the database server with java application, you must establish the connection with database, send SQL statements, and process the results. In the GTSS/Chrom-Quiz application, the instructor and the administrator can manage the database without going to the lower level of the database server.

5.5 Recompile

Any changing in the java files in the Chromatography engine requires the programmer to recompile using Javac from the command line. You can run it from the dos in the windows 2000 using this command:

```
C:/Javac chromatography.java
```

```
C:/dir
```

```
C:/chromatography.class
```

Once you recompiled java file, you should got the new file contain a bit code and the extension of this file is class, which is representing the bit code for

this java file. After you finished recompiling, you should put the classes back in the same directory of the GTSS package. Testing the GTSS project as a one unit is very important to make sure that every thing is working.

CHAPTER SIX

CONCLUSIONS AND FUTURE

DIRECTIONS

The GTSS/Chrom-Quiz system consists of two parts: the chromatography applet as a part of the GTSS project and Chrom-Quiz Web application as an evaluation tool. Java technology made it possible to integrate the GTSS and Chrom-Quiz system into one environment for teaching the liquid chromatography technique. Chrom-Quiz is very fast, reliable, and accessible through the Web. The system enables students to develop their understanding about the chromatography technique. The Chrom-Quiz system provides a guided tutorial for learning about chromatography.

6.1 Conclusions

The chromatography applet will allow students to conduct multiple experiments without being in the laboratory and without costly equipment and chemicals. The chromatography applet's will animate the chromatographic separation process and visually present the concepts of liquid chromatography technique. When embedded in the Chrom-Quiz System, the multiple-choice questions will guide the student to understand the effects of chromatographic variables on separation. Also, the

advantage of using GTSS/Chrom-Quiz is allowing the students to perform chromatography simulation before doing the actual experiment. The student can access the Chrom-Quiz through any Java-enabled Web browser. Every student will have a private account to access the Chrom-Quiz system and store his/her chromatography quiz score in the database. Students may repeat the chromatography simulation and take the chromatography quiz as many times as they wish. The student can choose the best score to be saved on the Chrom-Quiz database system. The instructor has the ability to create, edit and delete chromatography questions. The instructor can keep track of the students by progress accessing the student information. Also, the instructor can delete a student account to manage the database without going to the administrator level. Using Chrom-Quiz system is an important tool to enhance the student knowledge and student concepts about chromatography technique.

This master's project adds a new application engine to the GTSS structure (see Figure 39). The chemistry engine objects in the inner layer consist of the lineGraph and CherkersPanel classes. The chromatography application objects in the top layer are initiated from the chromatography class. The chromatography class is

responsible for using the chemistry engine to generate animation for the liquid chromatography technique. This project provided an interface to the WISE in order to build evaluation questions for the students. These interfaces can be reused by a developer to build any other discipline in the GTSS. The interfaces are included in the core objects of the GTSS set of tools. The Web address for the GTSS/Chrom-Quiz is:

<http://ias.csci.csusb.edu/chrom-quiz/index.html>

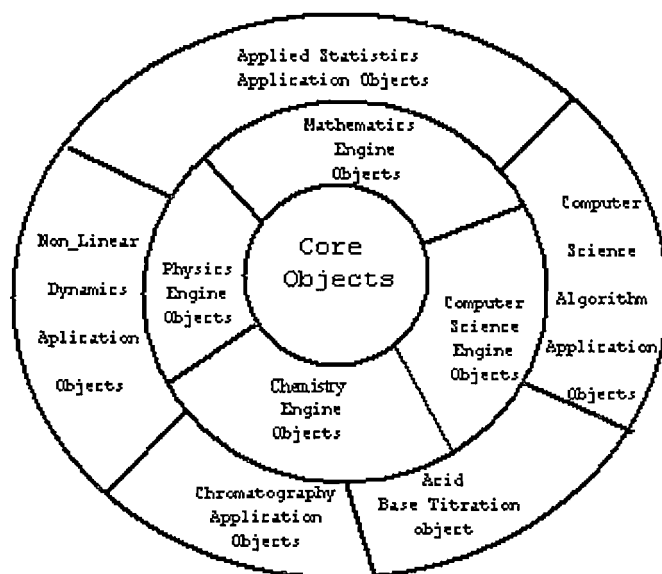


Figure 39. The New GTSS Layered Structure

6.2 Future Directions

Using the chemistry engine one can create a new applet to represent other chromatography techniques, such as, gas chromatography and column chromatography. It will

be very easy for a developer to design a new applet by reusing the code and the objects that were used in building the first chromatography applet model. In addition, we can update the liquid chromatography applet by adding new components to the chromatography Java file. So the chromatography applet can be expanded to cover most of the chemical compounds.

Provide display tables to instructors so that more components can be added conveniently by providing a computational function to calculate the speed of the different chemical compounds. In this way, the instructors can enter new components in the chromatography applet without computing their speeds outside of the system.

Test the system in an actual chemistry class to get feedback from the students and instructors for testing and improving the Chrom-Quiz system.

The quiz in this project contains only multiple-choice type of questions. In the future, we can add new question types like fill in the blanks and true or false questions. We can also change the number of choices for each question to allow flexibility in the number of choices in a multiple type of questions.

APPENDIX A
SIMULATION OF LIQUID
CHROMATOGRAPHY

SIMULATION OF LIQUID CHROMATOGRAPHY

This section explains how the calculations are done to get the speed of the different compounds. Based on correlation between "fit" values for hexane and ethanol, and the Kow of each (plot 1/Kow vs. 1/sol factor for hexane, ethanol; derived Kow is concentration ratio of Octanol and water. Sol is the solvent factor for compound. Nstat is the number of molecules in the stationary phase and Nmobile is the number of molecules in the mobile phase. Equation: sol factor = $Kow / (10.0 - 0.00067 * Kow)$

Generic Rate Equation

The generic rate equation derived from the chromatography theory. The equation that we used in the chromatography simulation applet is:

Rate = rate solvent front * (mole fraction in mobile phase) / (mole fraction in stat phase + mole fraction in mobile phase)

Rate = maxrate * $(1 / (1 + Nstat / Nmobile))$

Rate = maxrate * $(1 / (1 + (solfactor / Kfor\ compound)))$

Rate = maxrate * $K\ for\ compound / (K\ for\ compound + solfactor)$

maxrate = 6 for calculations

The following table shows the calculation of the soluble factor for each solvent that used in the chromatography simulation.

Solvent systems	Kow	Calculated sol factor
Hexane	12882.49552	9412.020126
10% EA/90% hexane	11594.7246	5195.852668
50% EA/hexane	6443.640909	1133.892728
dichloromethane	17.7827941	1.780400663
EA	4.786300923	0.47878363
50% EA/acetone	2.68087043	0.268135205
Acetone	0.575439937	0.057546212
50% acetone/ethanol	0.538313585	0.0538333
Ethanol	0.501187234	0.050120406

The following table shows how the size adjusted for the compounds that are used in the chromatography simulation.

Size factor = 1 for compact structures (single or bicyclic 4.3.0; 9-14 heavy atoms)

Size factor = 0.04 for xanthaphyll, beta-carotene (42 and 40 heavy atoms; extended structure)

Size factor = 0.025 for chlorophyll a (65 heavy atoms; large polycyclic structure)

Compounds	Kow	size adjusted K for compound
nicotinamide	0.426579519	0.426579519
Caffeine	0.851138038	0.851138038
acetaminophen	2.884031503	2.884031503
Acetanilide	14.45439771	14.45439771
Aspirin	15.48816619	15.48816619
Carvone	1174.897555	1174.897555
Naproxen	1513.561248	1513.561248
Xanthaphyll	6.60693E+14	4329.920581
Ibuprofen	9332.543008	9332.543008
chlorophyll a	7.4131E+16	11311.4966
Limonene	37153.52291	37153.52291
beta-carotene	4.16869E+17	2731995.192

The following table shows the rate of the three compounds Hexane, 10% EA/90% hexane, and 50% EA/hexane

	Hexane	10% EA/90% hexane	50% EA/hexane
Compound	Rate		
nicotinamide	0.000271925	0.00049256	0.002256399
Caffeine	0.000542537	0.000982705	0.004500424
acetaminophen	0.001837957	0.003328537	0.015222152
acetanilide	0.009200299	0.016645158	0.075522796
Aspirin	0.009857217	0.01783207	0.08085135
Carvone	0.665858141	1.106523578	3.053280925
Naproxen	0.83120222	1.353526195	3.430226766
xanthaphyll	1.890527986	2.727287623	4.75483367
Ibuprofen	2.987279973	3.854194179	5.349983458
chlorophyll a	3.274974055	4.111440214	5.453343227
Limonene	4.787255188	5.263858898	5.82230829
beta-carotene	5.979400317	5.988610544	5.997510781

The following table shows the rate of the three compounds Dichloromethane, Ethyl acetate, and 50% ethyl acetate/acetone

	Dichloromethane	Ethyl acetate	50% ethyl acetate/acetone
Compound	Rate		
nicotinamide	1.159719119	2.82701711	3.684213138
Caffeine	1.940624406	3.83994663	4.562628706
acetaminophen	3.709816844	5.14574496	5.48961734
Acetanilide	5.34200575	5.80762962	5.890724562
Aspirin	5.381396032	5.8200845	5.897894107
Carvone	5.990921557	5.99755593	5.998630992
Naproxen	5.992950498	5.99810262	5.998937257
xanthophyll	5.997533901	5.99933662	5.999628466
Ibuprofen	5.998855578	5.9996922	5.999827618
Chlorophyll a	5.999055764	5.99974605	5.999857775
Limonene	5.999712493	5.99992268	5.999956699
beta-carotene	5.99999609	5.99999895	5.999999411

The following table shows the rate of the three compounds Acetone, 50% acetone/ethanol, and Ethanol

	Acetone	50% acetone/ethanol	Ethanol
Compound	Rate		
Nicotinamide	5.2868	5.327661985	5.369
Caffeine	5.62003	5.643082839	5.666
acetaminophen	5.88262	5.890056275	5.898
Acetanilide	5.97621	5.977736789	5.979
Aspirin	5.97779	5.979217616	5.981
Carvone	5.99971	5.999725095	6
Naproxen	5.99977	5.999786604	6
Xanthaphyll	5.99992	5.999925404	6
Ibuprofin	5.99996	5.99996539	6
chlorophyll a	5.99997	5.999971445	6
Limonene	5.99999	5.999991306	6
beta-carotene	6	5.999999882	6

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