AC 2011-2501: USING WEB APPLETS TO STIMULATE LEARNING

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Using Web Applets to Stimulate Learning

Abstract

A series of web-based applets were developed to introduce students to a range of topics suitable for high school physical science, chemistry and physics classrooms. The applets were motivated by the authors' National Science Foundation (NSF) grant award, which focuses on the use of Computer Aided Molecular Design (CAMD) for the discovery of new compounds for various industrial applications. At the heart of the CAMD approach, students must fundamentally understand how data is reduced into correlations using linear and non-linear techniques and that a molecule's structure endows it with its properties and, hence, functionality in various applications. As a way of introducing such concepts to high school students, the PI's, in collaboration with a College-wide Research Experience for Teachers (RET) site, and a high school teacher, identified State mandated Science and Mathematics Standards that mapped to various skill sets required to learn and understand CAMD. These skills included understanding linear correlations and the concept that structure imparts property. Three applets were built and tested in the fall of 2010. These applets included one for conducting generalized linear relationships, one specialized for helping students to understand mass, volume and density and one to introduce students to the concept of structure-property relationships. The design strategy and methodology used is discussed as well as the architecture of the applets. Outcomes from the pilot test with high school students are also presented.

Introduction

Science and engineering are moving towards a discovery-based strategy that increasingly relies on the use of computational techniques¹. As our quantitative understanding of the physical world increases and as computer technology improves, becomes faster and has more memory capabilities along with computational algorithms that are robust and efficient, the application of computer aided model-based approaches to predict designs for structures, machines, electronics and even molecules becomes possible and practical. The authors engage in research that incorporates various computer aided model-based activities including developing models for physical phenomena such as chemical reactions², the behavior of complex processes³ and designing molecules for various applications⁴. As part of their ongoing National Science Foundation (NSF) grant entitled, "Controlling the Properties and Performance of Concrete Using Computer Aided Molecular Design"⁵, and in collaboration with a NSF Research Experience for Teachers (RET) site, they have developed a series of web-applets⁶ (web-based applications) that can be used by high school teachers or in introductory-level college courses, to introduce students to concepts associated with correlation and molecular structure-property (activity) relationships, both topics that are essential for conducting molecular design.

Research Experience for Teachers is an NSF initiative that:

“... supports the active involvement of K-12 teachers... in engineering research in order to bring knowledge of engineering and technological innovation into their classrooms. The goal is to... involv[e] the teachers in engineering research and helping them translate their research experiences and new knowledge of engineering into classroom activities⁷.”

The RET site at TTU is called RETainUS and is a multidisciplinary program focused on reintroducing manufacturing in its modern view, “a field full of challenging opportunities.” The program pairs faculty mentors from different departments with high school teachers. The teacher joins the mentor’s research group, develops a research question and for six weeks during the summer months conducts research, much as a graduate student or Research Experience for Undergraduate (REU) student would. During that time, the teacher also develops a lesson plan, using the Legacy Cycle pedagogy⁸ that will be implemented in the succeeding school year with his or her high school class. Figure 1 illustrates how the program at TTU works.

Figure 1. A conceptual image of how the RETainUS RET is structured.

This paper describes an RET experience wherein a single teacher worked with two faculty and the undergraduate and graduate students in their group to develop web applets as part of the Legacy Cycle lesson plan.

It is not up for debate, young people are “embedded” in a technological environment wherein their daily activities revolve around the use of cell/smart phones and related technologies, and that the business, medical, industrial, engineering, etc. workplace is becoming increasingly web

connected. Likewise, educational practices are now moving quickly to take advantage of web-based learning modalities⁹. And, while the use of web technologies as learning aids is yet debatable, studies do suggest that web-tools, including applets, appear to improve student learning measures including retention^{10, 11}. It appears that the community at large is moving towards increased utilization of web-based tools as part of a broader learning pedagogy. One study indicates, however, that web-applets need to be used in a constructivist learning environment¹¹. Constructivist learning theory suggests that people learn new things by “constructing” thought processes (schema) based upon their existing knowledge and understandings. The inquiry-based Legacy Cycle pedagogy used by the authors is one such constructivist learning pedagogy.

Background

The web applets and lesson plans described here are intended to introduce high-school or introductory-level college students to concepts associated with Computer Aided Molecular Design (CAMD) and in particular the concept and use of the Quantitative Structure-Property Relationship (QSPR). Scientists and engineers are frequently searching for a substance that has a particular property or they have a substance that they would like to know a certain property for. Rather than make a measurement, often times, it might be enough to estimate the property using some form of mathematical model first or to attempt to predict the structure that would produce a desired property. This approach is usually much more cost effective than running experiments. Once predictions have been made, experiments might be conducted to verify the validity of the projected behavior for targeted substances. Extracting information from a QSPR is one such CAMD strategy that enables this form of advanced computationally aided decision making.

The web applets are an embedded element of the broader lesson plans which apply the Legacy cycle pedagogy. The Legacy Cycle is a strategy that uses challenge questions to promote student driven inquiry. While the Legacy Cycle concept is explained in detail elsewhere¹², the basic elements include:

1. The challenge – a statement or question that provides an objective and motivation
2. Generation of ideas – considering how to address the challenge and possible approaches
3. Multiple perspectives – obtaining input from various sources; literature, others, etc.
4. Research and revise – conducting an experiment, doing some calculations
5. Test your mettle – testing your findings by some means
6. Go public – telling others what you found

A series of three applets and associated lesson plans were developed: (1) Linear Relationships; (2) Mass and Volume and (3) Structure Property Relationships. During the Fall of 2010, the

applets and lessons were beta tested in five individual classrooms/laboratories with 150 students at a single high school.

About the applets

The applets are structured in layers beginning with easily understood fundamentals that the students can read through and learn from. These layers, are implemented via a click on list of topics that open to new levels. As students move through the list and levels, they explore deeper levels of complexity within the subject. Some levels contain interactive modes that require student inputs, either experimental or conceptual. The models return responses including graphs and computed values, which are left deliberately uninterpreted. Interpretation is left to the students' own inquiry via the lesson plan.

Linear relationships

The *Linear Relationships* applet is a simple interface wherein students can input up to four x-y sets of data, plot them and retrieve the least-squares-best linear fits and R^2 values. This applet provides the template for the Mass and Volume applet, but is generalized for use with any x-y dataset.

Mass and volume

The *Mass and Volume* applet allows the student to explore the relationship between the amount of matter present and the amount of space that it takes up. The relationship between mass and volume for a substance depends on the mass of the particles that make up the substance and how much space the particles occupy. The relationship between mass and volume is therefore a *structure-property relationship*. The structure of the substance determines the property (mass-volume relationship) of the substance. Particles that are close together will take up less space than particles that are far apart. A substance that consists of massive particles that are close together will have a different mass and volume relationship than a substance that consists of less massive particles that are far apart. For a pure substance, the relationship between mass and volume is an intrinsic property. This means that the relationship between mass and volume will be the same for every sample of the substance and will be the same for any size sample. Mass and volume relationships are usually expressed as a ratio. A ratio is simply a way of expressing quantities relative to each other, for example, the ratio of mass to volume. This ratio is familiar to many students as the density of the material. With this lesson, teachers can help students to understand the material property of density and can introduce the concept of the structure property relationship in a context that most high school student are familiar with and will understand.

Structure property relationships

In this applet, the density, refractive index and viscosity of pure component organic substances are estimated using a molecular group-contribution based approach. A database of 25 compounds was assembled from which model parameters were estimated (see Appendix for list). The models take the following forms:

$$\rho = a_1 + a_2x_{Ring} + a_3x_{Cl} + a_4x_{OH} + a_5x_{Ester} + a_6x_{C=O} + a_7x_{COOH} + a_8x_C \quad (1)$$

$$n_D^{20} = b_1 + b_2x_{Ring} + b_3x_{Cl} + b_4x_{OH} + b_5x_{Ester} + b_6x_{C=O} + b_7x_{COOH} + b_8x_C \quad (2)$$

$$\ln\left(\frac{\nu}{M}\right) = A' + \frac{B'}{T} \quad (3)$$

$$A' = A_1 + A_2x_{Ring} + A_3x_{Cl} + A_4x_{OH} + A_5x_{Ester} + A_6x_{C=O} + A_7x_{COOH} + A_8x_C \quad (3.1)$$

$$B' = B_1 + B_2x_{Ring} + B_3x_{Cl} + B_4x_{OH} + B_5x_{Ester} + B_6x_{C=O} + B_7x_{COOH} + B_8x_C \quad (3.2)$$

where ρ = density, n_D^{20} = refractive index at 20 °C, and ν = kinematic viscosity, the a_i , b_i , and A' and B' are the correlation parameters and the x_i are the number of each of the i groups in the molecule; Ring (aromatic ring, delocalized bonding, e.g. benzene ring), Cl (chlorine), OH (hydroxyl), C=O (carboxyl), COOH (carboxylic acid) and C (total number of carbon atoms). Notably, Equation (3) is the group contribution model of Orrick and Erbar¹³ for viscosity. Multiple linear regression was used to find the best fit parameters for the models.

For teachers

Legacy cycle lesson plans

Lesson plans were developed to be used with the *Mass and Volume* and the *Structure-Property Relationships* applets. Lesson outlines are provided in the Appendix. A summary of the lesson and brief discussion is provided here for each.

Mass and volume

In this lesson, students are challenged to identify if an unknown soft drink is a diet or regular drink. The challenge is framed in the context of a shipment of unlabeled soda bottles with no indication of the drink type. Students are led through a guided inquiry Legacy Cycle that enables them to discover that density is a property that can be used for identification of the unknown. It turns out that diet soda has a distinctly different density than its regular counterpart (that made with sugar). Most labs on density will have students make a single measurement, e.g. measure the mass of a volume of liquid, then divide the mass by the volume to obtain the density. While

this activity will teach students that density is defined as mass divided by volume and if the instructor tells the student that it is an intrinsic material property that does not change with the extent of the material, i.e. the amount of material, then, it might be that the student will obtain some understand of what density is. However, it is doubtful that students will learn anything about quantitative structure property relationship (QSPR) theory from this form of exercise. Furthermore, the single point density measurement lab misses the opportunity to do much, much more. Having students explore the relationship between mass and volume by making three, four, or even more mass-volume determinations and then having them plot the data, offers the instructor the opportunity to make many more science standards connections and to introduce the concept of data correlation and the QSPR. When volume is plotted as a function of mass, the resulting linear proportionality constant is density. The Mass and Volume applet is a template for plotting and performing the linear regression. And, while it is just as “easy” to have students do this by hand, the applet is a way to introduce students to the concepts of graph interpretation and the use of technology which supplements their ability to make x-y plots by hand.

Structure-property relationships

Predicting the properties of substances is not a common topic in the high school chemistry and physics curriculum, however, it offers many opportunities for discovery-based lessons. This lesson places the students in a situation wherein they must identify an unknown pure component liquid from among a large number of possibilities. The lesson plan is appropriately titled, “What are These?” since it places the student in a hypothetical situation wherein they discover a number of unlabeled containers in a chemical storage cabinet along with a list of chemicals that had been stored there at one time. The Legacy Cycle in this case coaches students to use viscosity, density and refractive index as possible properties that might be used to determine what the unknowns are. In addition, since they have the list of possible chemicals, they can also determine what the properties for those chemicals are using a QSPR. The applet is a tool that they have at their disposal for this purpose.

Worksheets

A series of worksheets are provided in the Appendix which can be used to help students to organize their data. The instructor might choose to use the worksheets or to have students think about how they might organize and record their data without the worksheets.

Connecting to state science and math standards

While understanding quantitative structure property relationships is not explicitly listed as a science standard in any state that the authors know of, the activities are rich with science standards connections. A mapping of these activities to the science and math standards for the

State of Tennessee is provided on line⁶. The *Mass and Volume* activity was mapped to 39 individual standards while the *Structure Property Relationships* activity was mapped to 27 standards cutting across both the math and science goals.

Beta test with students

The *Structure Property Relationships* activity was beta tested with 150 general chemistry students, predominantly 10th graders at Cookeville High School (CSH), Cookeville, Tennessee. The demographics at CSH are 15% minority, 10% special education, 27% economically disadvantaged and 1% English language learners; these figures nominally represent the subject student body. While no controlled assessment was conducted, the outcomes were measured in terms of how well the students were able to conduct various portions of the activity and student perceptions. Students worked in small teams of four to six. All thirty-three student teams correctly encoded simple organic compounds in terms of functional groups. Twenty-five of the 33 teams successfully identified their unknown; those that did not made errors in their laboratory measurements.

For the density project, students were assessed and graded based on their lab worksheets. For the organic unknown project, students were assessed based on a formal, written lab report completed in groups and were also assessed based on their group presentations of their unknown identification. These two assessments were combined to assign a grade to each group. Their lab technique was assessed based on their lab worksheets but was used as a formative assessment and was not part of their grade.

In a pre-course survey 57% of the students said that they enjoy science while 22% said that they do not. In a post-course survey 63% said that they enjoy science with 17 % saying that they do not. While these outcomes and statistics are by no means conclusive in any way, it does suggest that the activity improved student perceptions of science and that they were able to use the new tools (applets) to accomplish a fairly complex objective.

Summation

Collaboration between two NSF funded grants produced a series of web applets and associated lesson plans for the introduction of structure property theory in high school science curricula. The lesson plans focus on a pair of activities, one an introductory activity that explores the mass-volume relationship and density and the other that uses group contribution concepts to predict the viscosity, density and refractive index of pure organic liquids. The project was conducted under an RET site program and involved a science teacher, two undergraduate research students and two faculty mentors. The lessons were beta tested in five general chemistry classes with 150 students working in small teams. The results suggest that the lessons are effective at teaching the

target concepts and content and that the use of the Legacy Cycle in combination with the web applets may contribute to improving student perceptions of science.

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Appendix

List of Compounds Used to Develop Group Contribution Models

Mass Volume

LEGACY Cycle

Lab Purpose and Procedures

Lab Worksheet – Mass and Volume

Follow-Up Questions

Lab Worksheet and Procedures – Finding the Density of a Liquid

What are these?

Worksheet – Unknown Compounds

Worksheet – Structure and Functional Groups

Lab Procedures – Using the Refractometer

Lab Procedures – Using the Viscometer

List of Compounds Used to Develop Group Contribution Models

1. Ethylene glycol
2. Acetone
3. Ethanol
4. 1-Propanol
5. Methanol
6. Carbon tetrachloride
7. Acetic acid
8. Hexane
9. 1-Pentanol
10. 1-Butanol
11. Toluene
12. Benzene
13. Ethylbenzene
14. Propylbenzene
15. Pentane
16. propanoic acid
17. butyl acetate
18. methyl acetate
19. propyl acetate
20. ethyl acetate
21. butyric acid
22. Valeric acid
23. methyl benzoate
24. ethyl benzoate
25. heptane

Mass and Volume

LEGACY Cycle

This Legacy Cycle is planned for 55 minute class periods.

Day 1

Challenge Question: You have a truckload of unlabeled soft drinks in two liter bottles. You need to determine whether the beverages are regular or diet and must have *hard* (quantitative and defensible) data to support your choice.

Generate Ideas: Students will *Think-Pair-Share* what they *Know and Need to Know* to answer the question. Teacher may record ideas on the board or on a transparency to be used later.

Multiple Perspectives: Students will examine labels of regular and diet drinks and determine what differences are there. How these differences may affect the properties of the soft drinks will be explored.

Research and Revise: Students will be introduced to mass-volume relationships; instruct them to open the Mass and Volume applet and read "Mass Volume Relationships."

Day 2

Conduct Experiment: Students will complete the experimental elements of the Mass-Volume lab.

Use the Mass-Volume Applet: Students will input mass and volume data they determined experimentally. The applet will generate a graph of mass vs. volume, a line of best fit, and the equation for the line. Students can determine the slope of the line can using the "rise over run" formula or from the equation generated by the applet.

Test Your Mettle: Students will fill out a lab report that will explore their understanding of the mass and volume relationship.

Day 3

Research and Revise: The teacher should provide a brief *lecture* on mass-volume relationships, introduce the term "density," and explore the idea that the slope of the mass-volume line has units and a physical meaning. The teacher may also briefly explain the significance of the R^2 term. Teacher will demonstrate how to calculate density using mass and volume, emphasizing the proper use of units and significant figures.

Apply what Your Have Learned: Return to the *Challenge Question* and the *Know and Need to Know* list. Students should now be able to suggest a method for determining the identity of the unknown.

Guide the students' inquiry as necessary to develop and design their own experiment to determine the identity of the unknown, including appropriate controls.

Day 4

Test your mettle: Students will return to the lab and attempt to identify their unknown based on a density comparison to that known for other soft drinks; to be provided by the teacher. Students may use the applet again to plot their data, this time comparing their unknown to known values, or they may calculate the densities by hand.

Go public: Each group has a different unknown to identify. Students will informally present their findings to the class using whiteboards and explain how they identified the unknown.

Mass and Volume

Lab Purpose and Procedures

Purpose: To illustrate the relationship between mass and volume.

In this lab, you will measure the mass and volume of several samples of different materials. You will then use a computer applet to generate a graph that will illustrate the mass and volume relationship of each of the materials.

Procedure:

1. Obtain samples of 4 different materials. Each material is available in 4 different sample sizes. Take all 4 sample sizes with you to your lab table. Record the names of your materials in your data tables.
2. Use a balance to determine the mass of each sample to the nearest 0.1 g. Record the masses in your data table. If you are using an electronic balance, be sure to press the TARE button to return the balance to 0.0 g if needed.
3. Use a graduated cylinder to determine the volume of each sample by water displacement.
 - a. Use a 100 mL cylinder.
 - b. Put about 40 mL of water in the cylinder. Accurately record the volume of water to the nearest 0.5 mL in your data table. Remember to read the volume at the bottom of the meniscus!
 - c. Carefully slide the sample into the water (do not splash out any water or you will have to start over.) Accurately record the new volume of water to the nearest 0.5 mL in your data table. The difference between the two volume measurements is equal to the volume of your sample. Calculate the volume of your sample and record it in your data table.
4. When you have determined the mass and volume of all the samples, dry the samples and return them to the teacher's table.
5. Enter your data into the computer. Reopen the applet you used yesterday and click on the button that says "Mass and Volume Data and Graph." Enter the material name and your mass and volume data into the spaces provided.
6. Under the graph, click on the buttons to display your data in the graph. Write the equation for the line and the R^2 value for each material in your data table.

Mass and Volume

Lab Worksheet

Material 1: _____

Sample	Mass (g)	Volume in cylinder without sample (mL)	Volume in cylinder with sample (mL)	Volume of Sample (cm ³)
1				
2				
3				
4				
Line equation:				R ² :

Material 2: _____

Sample	Mass (g)	Volume in cylinder without sample (mL)	Volume in cylinder with sample (mL)	Volume of Sample (cm ³)
1				
2				
3				
4				
Line equation:				R ² :

Material 3: _____

Sample	Mass (g)	Volume in cylinder without sample (mL)	Volume in cylinder with sample (mL)	Volume of Sample (cm ³)
1				
2				
3				
4				
Line equation:				R ² :

Material 4: _____

Sample	Mass (g)	Volume in cylinder without sample (mL)	Volume in cylinder with sample (mL)	Volume of Sample (cm ³)
1				
2				
3				
4				
Line equation:				R ² :

Mass and Volume

Follow-Up Questions

1. Do all of the materials have the same relationship between mass and volume? How did you determine this?
2. If you had one piece of each material and all the pieces were the same mass, would they all have the same volume? How did you determine this?
3. If you had one piece of each material and all the pieces were the same volume, would they all have the same mass? How did you determine this?
4. How can you determine the slope of a line? Is the slope of a straight line the same at all points on the line?
5. What is the formula for the equation of a line? What does it mean if there is no “b” term?
6. How can you determine the slope of a line using the equation found by the applet?
7. What is a ratio?
8. What does the slope of the line tell you about the mass and volume relationship of the material?
9. Use the graph to determine the mass of each material that would be contained in 1.0 cm^3 of the material.

Mass and Volume

Lab Procedures for Finding the Density of a Liquid

1. Place a clean, dry graduated cylinder on the balance. Record the mass to the nearest 0.1 g. You only need to obtain this value once.
2. Place the liquid into the graduated cylinder. For the most accurate results, use a dropper pipet to bring the meniscus exactly to one of the markings on the cylinder. Obtain the mass of the cylinder plus the liquid.
3. Record the mass of the liquid plus the cylinder in your data table. The difference between the mass of the cylinder plus the liquid and the mass of the cylinder alone is the mass of your liquid.
4. Record the volume of the liquid to the nearest 0.5 mL and record in your data table. The liquid can be poured down the sink and the graduated cylinder can be rinsed with water and shaken out between samples.
5. Calculate the density of the liquid and record in your data table.
6. Repeat the above steps and average the densities to improve your accuracy.
7. Rinse the graduated cylinder and clean up your lab station.

Sample	Mass of Cylinder	Mass of Cylinder Plus Liquid	Mass of Liquid	Volume of Liquid	Density of Liquid	Average Density
Regular Soft Drink						

Diet Soft Drink	-----					

Your Unknown	-----					

Based on the above data, determine the identity of your unknown.

Be prepared to present your findings to the class, to defend the identification of your unknown and to answer the following questions.

- What were your known soft drinks (brand, flavor)?
- What were their densities? Can you explain the procedure you used to determine this?
- What was the density of your unknown?
- How did the density of your unknown soft drink compare to the density of your known soft drinks?

What are these?

LEGACY Cycle

This Legacy Cycle is planned for 55 minute class periods.

Day 1

Challenge Question: You are a scientist working in a lab. You find an old cabinet with eight* unlabeled chemical bottles inside. Also inside the cabinet is a list of many compounds that have been stored in the cabinet. How can you determine the identity of the unknown chemicals?

Generate Ideas: Instruct student to *Think-Pair-Share* what they *Know and Need to Know* to answer the challenge.

Multiple Perspectives: Students should read the *Molecular Structure, Functional Groups, Properties, Quantitative Structure-Property Relationships*, and *Mathematical Modeling* sections of the applet. Teacher should review information with students to ensure understanding.

Day 2

Research and Revise: Teacher should review the material presented the previous day. Demonstrate how to determine functional groups from skeletal formulas. Hand out the *Compound Worksheet*. Instruct students to examine the possible compounds and to determine the functional groups that are present. Students will enter functional group data into the applet and generate data on viscosity, refractive index, and density. Students should determine that they will need to make experimental measurements to check their unknowns for refractive index, viscosity, and density.

Day 3

Research and Revise: Students will go to the lab to test their unknowns for refractive index, viscosity, and density.

Test Your Mettle: Students will identify their unknowns using their lab data. Students will complete a lab report.

Day 4

Go Public: Students will prepare and present posters or whiteboards that illustrate the structure of their identified compound with functional groups and compare their experimental data with the data generated by the applet.

* Fewer compounds can be used successfully in this activity, but each group will not have a unique unknown.

What are these?
Worksheet – Unknown Compounds

Name: _____ Date: _____ Period: _____

Viscosity, Refractive Index, and Density Lab

Viscosity

Time = (minutes × 60) + (seconds) _____

Viscosity = Time in seconds × Viscometer Constant

Time in Seconds	Viscometer Constant	Viscosity (cSt)

Refractive Index

Readings: _____

Density

Density = Mass ÷ Volume

Mass of Sample (g)	Volume of Sample (mL)	Density of Sample (g/mL)

Conclusions

Based on the viscosity, refractive index, and density you obtained, identify your unknown.

Draw the skeletal formula of your unknown.

Identify the functional groups of your unknown.

What are these?

Worksheet – Structure and Functional Groups

Name: _____ Date: _____ Period: _____

1-Butanol Molar Mass ____g/mol		Health - 1 Flammability – 3 Instability – 0	
Functional Groups					
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid
Properties					
Viscosity		Density		Refractive Index

1-Pentanol Molar Mass ____g/mol		Health - 1 Flammability – 3 Instability - 0	
Functional Groups					
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid
Properties					
Viscosity		Density		Refractive Index

Acetic Acid Molar Mass ____g/mol		Health - 2 Flammability – 2 Instability - 2	
Functional Groups					
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid
Properties					
Viscosity		Density		Refractive Index

Butyl Acetate Molar Mass ____g/mol		Health - 1 Flammability – 3 Instability – 0		
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity			Density		Refractive Index	

<div><div><div><div><div></div><div></div><div></div><div></div></div><div><div><div>Cl</div><div>Cl</div><div>Cl</div><div>Cl</div></div></div></div></div></div>	<div>Carbon Tetrachloride</div> <div>Molar Mass ____g/mol</div>	<div>Health - 3</div> <div>Flammability – 0</div> <div>Instability - 0</div>				
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity		Density		Refractive Index

<div>Ethanol</div> <div>Molar Mass ____g/mol</div>			<div>Health - 1</div> <div>Flammability – 3</div> <div>Instability - 0</div>	
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity		Density		Refractive Index

Propyl Acetate		Health - 2 Flammability – 3 Instability - 0		
		Molar Mass ____g/mol				
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity			Density		Refractive Index

<div>Heptane</div> <div>Molar Mass ____g/mol</div>			<div>Health - 1</div> <div>Flammability – 3</div> <div>Instability - 0</div>	
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity			Density		Refractive Index

<div>Propylbenzene</div> <div>Molar mass ____g/mol</div>			<div>Health - 1</div> <div>Flammability – 3</div> <div>Instability - 0</div>	
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity		Density		Refractive Index

<div>Toluene</div> <div>Molar Mass ____g/mol</div>			<div>Health - 2</div> <div>Flammability – 3</div> <div>Instability - 0</div>	
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity		Density		Refractive Index

<div>1-Propanol</div> <div>Molar Mass ____g/mol</div>			<div>Health - 1</div> <div>Flammability – 3</div> <div>Instability - 0</div>	
Functional Groups						
Delocalized/ Benzene Ring	Chlorine	Hydroxyl	Ester	Carbonyl	Carboxylic Acid	Carbon Count
Properties						
Viscosity		Density		Refractive Index		

What are these?

Procedures

Using the Refractometer

Read all directions before starting! Be very careful with the refractometer- it is expensive!

Image taken from <http://www.misco.com/products/PA202.html>.

1. Rinse the well of the refractometer with distilled water before use. Gently shake the water out and blot (don't rub) the well dry with one of the special wipes (KimWipes) on the lab bench. Don't use a paper towel.
2. Place a few drops of your sample into the well. Press "Go."
3. The refractometer will give you the refractive index of your sample. Record this value in your data sheet.
4. Rinse the well of the refractometer with distilled water and blot dry with one of the special wipes.

What are these?

Procedures

Using the Cannon-Ubbelohde Viscometer

Read all directions before starting! Be very careful with the viscometer- it is expensive!

1. Clean the viscometer with distilled water before use. Remove the viscometer from the clamp. Fill the large bulb with distilled water and gently invert the viscometer to rinse it. Use the red pipet bulb on the smaller tube of the viscometer to suction water into the small bulbs to rinse them. Pour the water out of the viscometer and use the red pipet bulb to force any leftover water out of the viscometer.
2. Rinse the viscometer with a very small amount of the sample you will be measuring. Use a funnel to pour a very small amount of sample into the large bulb. Gently invert the viscometer to rinse it. Use the pipet bulb to suction sample into the small bulbs to rinse them. Pour the sample into the waste beaker in the fume hood. Use the pipet bulb to force any leftover sample out of the viscometer.
3. Clamp the viscometer to the ring stand using the finger clamp.
4. Add a small amount of your sample to the large bulb using a funnel. You do not need to fill the large bulb more than $\frac{1}{2}$ full. Use the pipet bulb to suction sample up into the small bulbs.
5. Take the pipet bulb off of the viscometer. You will notice that your sample begins to drain out of the top bulb. Watch it carefully.
6. **Start** the stopwatch **immediately** once the meniscus of your sample reaches **line 1**. Continue to watch the sample carefully.
7. **Stop** the stopwatch **immediately** once the meniscus of your sample reaches **line 2**. Record the time it took for your sample to pass between the two lines on your data sheet. If you did not start or stop the stopwatch at the right times, you will need to suction sample into the top bulb and try again.
8. When you have a good reading of the time it takes the sample to pass between the lines, empty the viscometer into the waste beaker in the fume hood. Use the pipet bulb to force any leftover sample out of the viscometer. Rinse the viscometer with distilled water like you did in step 1. Return the viscometer to the clamp.
9. The time multiplied by the viscometer constant equals the viscosity. You can find the viscometer constant on the card on the lab table next to the viscometer.

Bibliography

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- ¹ Atkins, D. E., Droegemeier, K. K., Feldman, S. I., Garcia-Molina, H., Klein, M. L., Messerschmitt, D. G., Messina, P., Ostriker, J. P., and Wright, M. H., (2003), "Revolutionizing Science and Engineering Through Cyberinfrastructure," Report of the National Science Foundation Blue-Ribbon Advisory Panel on Cyberinfrastructure.
- ² Biernacki J. J. and Xie, T., (2011), "An Advanced Single Particle Model for C₃S and Alite Hydration," J. Am. Cer. Soc., in press.
- ³ Shanmugasundaram, S., Biernacki, J. J., and Subramanian, R., (2005) "Variation in Boron Doping by Planar Diffusion - A Comparative Study of Computational Hydrodynamics and Experimental Observations," Mat. Sci. Tech., 21(9) 1103-1110.
- ⁴ Visco, D. P., (2010), "Computer-Aided Molecular Design: Inverse Design," Chapter 9 in "Handbook of Cheminformatics Algorithms", ed. J. L. Faulon and A. Bender, CRC Press. London.
- ⁵ Biernacki, J. J., and Visco, D. P., Jr. (2009), "RUI: Controlling the Properties and Performance of Concrete Using Computer Aided Molecular Design," National Science Foundation, Grant Proposal No. CMMI-0928539.
- ⁶ Biernacki, J. J., (2011), "Web tools for research and education," <http://blogs.cae.tntech.edu/jbiernacki/>, accessed on January 8.
- ⁷ Research Experience for Teachers (RET) in Engineering and Computer Science, National Science Foundation, Program Solicitation NSF 11-509.
- ⁸ Schwartz, D., Brophy, S.P., Lin, X. and Bransford, J.D., (1999) "Software for Managing Complex Learning: Examples from an Educational Psychology Course." Educational Technology Research and Development, 47 (2), 39 -58.
- ⁹ Shotsberger, P. G. and Vatter, R., (2001), "Teaching and Learning in the Wireless Classroom," Computer, 34(3), 110-111.
- ¹⁰ Dinov, I., Sanchez, J., and Christou, N., (2008), "Pedagogical Utilization and Assessment of the Statistic Online Computational Resource in Introductory Probability and Statistics Courses," Computers and Education, 50(1), 284-300.
- ¹¹ Zhou, G., Brouwer, W., Nocente, N., and Martin, B., (2005), "Enhancing Conceptual Learning Through Computer-Based Applets: The Effectiveness and Implications," J. Interactive Learning Research, 16(1), 31-49.
- ¹² Schwartz, D. L., Lin, X., Brophy, S., and Bransford, J. D., "Toward the Development of Flexibly Adaptive Instructional Designs," Chapter 9 in Instructional-Design Theories and Models – A New Paradigm of Instructional Theory, Volume II, ed. C. M. Reigeluth, Lawrence Erlbaum Associates, Mahwah, New Jersey (1999).
- ¹³ Reid, R.C., Praunitz, J.M., Poling, B.E., (1975), "The Properties of Gases and Liquids," McGraw-Hill, New York.