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ChemLab Simulations

ChemLab is an interactive simulation of a chemistry lab. Common Lab equipment and procedures are used to simulate the steps involved in performing a chemistry lab experiment. Each lab simulation is contained in a separate simulation module, thus many different labs are possible using a common lab interface. A lab simulation module contains code and resources, such as chemical list, indicator list, available menu options and instructions specific to each lab. New lab modules can be added to ChemLab by copying them to the program directory. These lab modules are in fact extensions of the main ChemLab program, which is basically a common interface for them.

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Selecting a Lab Simulation:



A lab module is selected at start-up and when a new file is created or by selecting the lab option. The simulation dialog box presents a list of available labs and a short description of each one. To select a lab, click on the title of the lab you wish to perform and press OK. Clicking cancel will load the generic lab simulation.

When an existing file is opened it automatically loads the appropriate lab module. If that lab is not available a generic lab module is loaded which allows the viewing of the file.

In addition to selecting simulation modules, the user may also want to create their own labs using a Lab Wizard tool. These Lab Wizard tools can be viewed by selecting the Lab Wizards tab on the simulation dialog box. Selecting a Lab Wizard will take the user through the step-by-step process of creating a new custom lab called a UDL (User-Defined Lab) simulation. The stoichiometry Lab Wizard may be launched directly from the ChemLab by selecting Create New UDL under the File Menu. These UDL simulations will then appear in the list of available lab modules. The UDL file name will appear in the UDL file column. Once you have opened a UDL, it may be edited from ChemLab by selecting Edit UDL file under the File Menu.

Getting Started

When ChemLab is started or a new file is created the simulation dialog box will open. From this dialog box pick a simulation module to load. This will load the text window with the instructions necessary to perform the lab. Read the lab introduction in the introduction text window. The introduction will explain the basic science behind the lab. After reading the lab introduction read the procedure. To select the procedure click the procedure tab above the text window. In the procedure you will find the basic steps to complete the lab, you should first read the procedure completely before attempting the lab. If you are not sure how to perform a certain action check the lab manual or help for directions. Then perform the lab following the steps in the procedure. While performing the procedure you can record your observations in the observation text window, these will be saved in the ChemLab file.

The Organization of ChemLab

ChemLab consists of two windows, a text and Lab window, divided by a splitter bar. The Lab window displays the animated lab simulation. Objects in the form of lab equipment are added to this window. These objects can be added and acted upon by using the Chem toolbar or the main menu commands.

The text window serves as the center for textual documentation in ChemLab. It is divided into 3 windows; A read-only introduction and lab procedures, and a user writeable observation window. These windows are selected by pressing the text tab bar, located just above the text window.

The observation window allows the user to perform paragraph and character level formatting. These formatting options can be selected using either the text Toolbar, located just above the text window, or by using the text edit menu commands found in the edit main menu.



Lab equipment

Lab equipment is added to the Lab window by either selecting from the chem toolbar, equipment menu or additionally lab equipment can also be added through the chemicals dialog box by specifying a new lab container.

ChemLab provides the following pieces of lab equipment:

Beaker

Beaker : a wide mouth, thin walled containers with a projected lip used widely in laboratory chemistry. ChemLab provides a 100ml, 250ml and 600ml beaker. They can be added to the lab space by pressing the toolbar beaker button (100ml), selecting the 100, 250 or 600ml menu items from the equipment menu.



Buchner funnel

Buchner funnel : a funnel with a flat circular base perforated with small holes used for filtering with suction. In ChemLab a buchner funnel is added by first selecting an erlenmeyer flask and then picking the buchner funnel from the toolbar, equipment menu. To remove the funnel, do the same. If any solid is present in the filter a dialog box will appear asking whether you wish to discard or keep and place it another container.



Bunsen Burner

Bunsen burner: a gas burner used in laboratories. Consists of a metal tube with a valve for controlling the air-fuel mixture. In ChemLab the bunsen burner is added by selecting the bunsen burner button from the tool bar, equipment menu. If a container is selected when the bunsen burner button or menu item is selected a burner will be added just below the selected container. Lab equipment containers, which allow heating, that are place directly above a bunsen burner, will receive a fixed amount of heating from burner. The amount of heat transfer by a bunsen burner can be varied by changing the burner heat in the equipment option dialog box.



Buret

Buret: a graduated glass tubes with a stopcock valve used for transferring precisely measured liquid volumes. Used in volumetric analysis in laboratory chemistry. In ChemLab a 10ml and 50ml buret are provided. They can be added to the lab space by pressing the toolbar buret button, selecting the buret from the equipment menu.



A titration dialog box is opened when a new buret is added. The titration dialog box is used to control the rate of flow leaving the buret. A slider control in the dialog box labeled stopcock is used for this purpose. If an existing buret is selected when the buret button or menu is pressed no new buret will be added, rather the titration dialog box will then refer to the previously selected buret. To identify which buret the titration dialog box refers to; the buret's label value is added to the dialog box's menu bar. Note, only one titration dialog box can be opened at a time. The titration dialog box also updates the current volume of the buret to the nearest tenth of a ml and can be used to record the start and end-points of a titration.

Calorimeter

Calorimeter: is an instrument for determining the amount of heat evolved, transferred or absorbed. In ChemLab it consists of a closed insulated vessel with a thermometer. To add a calorimeter to ChemLab select the calorimeter menu option in the Equipment main menu. The calorimeter has a volume of 250ml and will be open when first added. To close a calorimeter, select it and press the thermometer tool bar button. This will add both a thermometer and a cork top to calorimeter. Doing this a second time will remove the thermometer and open the calorimeter. Note: the calorimeter will only be available for those experiments in which it is used. So the menu option will often appear grayed out.



Erlenmeyer Flask

Erlenmeyer Flask: a flat base conical flask with a narrow neck. ChemLab provides a 100ml and 250ml erlenmeyer flasks. They can be added to the lab space by pressing the toolbar erlenmeyer flask button, selecting erlenmeyer flask from the equipment menu.



Evaporation Dish

Evaporation Dish: is short wide mouth container with thick walls. ChemLab provides an evaporation dish with a volume of 100ml. They can be added to the lab space by pressing the toolbar evaporation dish button, selecting the evaporation dish from the equipment menu.



Florence flask

Florence flask: is a round container with a long neck and narrow mouth. ChemLab provides an florence flasks with a volume of 100ml. They can be added to the lab space by pressing the toolbar florence flask button, selecting the florence flask from the equipment menu.



Graduated cylinder

Graduated cylinder: is a tall cylindrical container with a finely marked scale, used for precisely measuring out liquid volumes. In ChemLab a 10ml and 50ml graduated cylinder are provided. They can be added to the lab space by pressing the toolbar graduated cylinder button (100ml), selecting the graduated cylinder from the equipment menu.



Stirring Rod

Stirring Rod: is a glass rod used for mixing. ChemLab allows the addition of a stirring rod for mixing to selected lab containers with some contents. The stirring rod may be added to a single selected item by pressing the stirring rod button on the toolbar, selecting stirring rod from the equipment menu. A user can also remove an existing stirring rod from a container by this same process. The stirring rod will remain in a container for only a few seconds; to continue stirring the user must re-select the stirring rod.



Test Tube

Test Tube: a plain or lipped thin glass tube closed at one end. ChemLab provides an test tube with a volume of 50ml. They can be added to the lab space by pressing the toolbar test tube button, selecting the test tube from the equipment menu.



Thermometer

Thermometer: is a instrument for measuring temperature, it consist of a closed narrow graduated tube with a bulb at one end. The tube contains a liquid, such as mercury, whose volume varies with temperature. Temperature is indicated by the height of the mercury column within the thermometer. ChemLab allows the addition of a thermometer to selected lab containers. The thermometer may be added to a single selected item by pressing the thermometer button on the toolbar, selecting thermometer from the equipment menu. A user can also remove an existing thermometer from a container by this same process. The recorded temperature is indicated by the height of the liquid in the tube and additionally by a text field at the top of the thermometer. The scale can be changed from Kelvin, Celsius or Fahrenheit by selecting the temperature scale setting in the equipment options dialog box.



Watch glass

Watch glass: is a short circular glass container, used for measuring out solids and other miscellaneous tasks in the lab. ChemLab provides an watch glass with a volume of 50ml. They can be added to the lab space by pressing the toolbar watch glass button, selecting the watch glass from the equipment menu.



Weighing scale

Weighing scale: are instruments used for weighing mass. ChemLab does not provide weighing scales but instead will show the sample weight in grams (that is the weight of only the contents of a container) of a selected container in a highlighted text field below the container. The sample weight may be added to a single selected item by pressing the scales button on the toolbar, selecting scales from the equipment menu. A user can also remove an existing sample weight from a container by this same process.



Using the mouse

ChemLab uses the mouse to select lab equipment for a number of actions:

Picking a single piece of lab equipment, either by single mouse click or dragging (holding down the mouse button while moving the mouse). Selecting a piece of lab equipment allows adding chemicals, water, thermometer, scale, stirring rod, bunsen burner, a funnel to a flask and decanting or pouring.



Double clicking the mouse

Double clicking the mouse button on a piece of lab equipment will open the chemical properties dialog box .

Double clicking on the label of a piece of lab equipment allows it to be edited.

Selecting two or more objects

To select two or more lab objects, drag the mouse around the objects while holding down the mouse button, then release the mouse key. A selection rectangle will then enclose the selected objects.

Combining and Removing Equipment

Selecting 2 pieces of lab equipment, which fit into each other, allows combining of lab equipment (arrange menu). Combining places one piece of lab equipment into another, this can be used to arrange a cooling or hot water bath. To remove two previously combined pieces of lab equipment select the combined object and select the remove menu option from the arrange menu.



Selecting 2 or more objects also allows grouping of objects together.

ChemLab Procedures

Positioning Lab Equipment

ChemLab tries to create the feel of a lab by using the position of certain lab equipment relative to other lab equipment. This is seen in decanting, or pouring, titration and heating with the bunsen burner.

Pouring/decanting

Pouring or decanting, involves selecting a piece of lab equipment, positioning its left side over the receiving container and selecting the decant button from toolbar or decant/pour menu item from the procedures menu. Note: liquid is first transferred in this process, to allow separation.



Heating

Similarly to heat an object with a bunsen burner, position the burner under that object.



Adding Chemicals

To add chemicals to a container first select the container and then select the chemicals button from the toolbar or chemicals menu item from either the main menu. This will open up a chemicals dialog box. The chemicals dialog box allows the users to add chemicals to the selected item or add chemicals to a new item. It will also allow the user to change the selected containers size and type. Select the desired chemical from the chemicals drop-down combo box. Enter the desired mass or volume of chemical needed and press OK.



Adding Indicators

Indicators are substances that signify the completion of a chemical reaction with a color change. To add an indicator to a piece of lab equipment, select it and then press the indicator menu option in the Chemical main menu. This will open a dialog box which list available indicators and their color change characteristics. Not all labs use indicators so this menu will often appeared grayed.

For those labs that do use indicators, select the desired indicator from the list of available indicators and enter the number of drops to add (from 0-10) and press OK. Indicators are generally ignored by ChemLab except to flag a Chemical reaction, so they will appear to have no weight or volume.



Adding Water

Water is added to a selected lab item by using either the toolbar water button or the water dialog box. To open the water dialog box, select the water menu item in the chemicals menu. Water may also be added through the Chemicals dialog box. The toolbar button will only add water at room temperature to a selected item to the next graduation on the container. The water dialog box also allows the users to add ice water, which is used to create ice baths. The water dialog box also only adds water in increments.



Adding a Label

ChemLab allows a user to add a label to a lab container, along with a short annotated note. By selecting a lab container lab and then selecting the label menu item in the procedures menu or by double clicking on the container's label area. This will open up the label dialog box, which allows the user to enter a 2 letter label, which is visible on the container and a short annotated note, which can be viewed from the label dialog box.



Chemical Properties Dialog Box

The Chemical Properties dialog box shows the current chemicals and their states in a piece of lab equipment.



Saving files

Lab experiments may be saved to file for latter use (file kind: ChemLab document). To save a file a user can select the toolbar file button, or file's menu save or save as menu selections.

Printing Files

ChemLab files may be printed by selecting the print toolbar button or by selecting the print menu in the file main menu. Printing will print the recorded lab observations.

Setting Options

ChemLab allows the setting of a number of options including: equipment options, current lab module, and window settings. These options are available under the options main menu.

Equipment options are set in the Equipment option dialog box. These options include the settings for the heat transferred by the bunsen burner, the size of the text font used in main lab window graphics; such as the equipment label, and the setting for the temperature scale used. These options once set are preserved until changed again.

Window option settings including whether both the main lab window and the text window are visible or only the lab window. This option can be set by selecting the toolbar button or the "Both lab & text" and "Lab Only" main menu options.

Warnings

Lab instructions included with ChemLab have been modified and simplified for purposes specific to ChemLab. They are not suitable for use in an actual lab setting and should not be used as a substitute for lab documentation and instructions developed for actual experimentation.

Feedback

Please send us your comments on this software, bugs, other problems, suggested improvements, and experiments you think could work in this format.

Our e-mail address is :

info@modelscience.com

Also check out the Model Science Web Site for new developments, down-loadable software and product information:

<http://www.modelscience.com>

You may launch your web browser by selecting Model Science Web Page from the Help Menu.

Lab Wizard

The Lab Wizard is a ChemLab tool used to design chemistry lab simulations. Although ChemLab comes with a variety of lab modules, such as an acid-base titration, you need not limit your work to these pre-fabricated experiments. Lab Wizard will translate your labs into ChemLab modules called User Defined Lab (UDL's) by asking you to supply it with chemical data and reaction formulas. These UDL files can then in turn be traded and exchanged among your colleagues. Model Science Software will be glad to post your lab simulations for you at their web site. Before you begin using the Lab Wizard, you should prepare the following:

- (1) Introduction, Procedure, and Observations RTF files.
- (2) a list of chemicals (reactants and products as well as all intermediate chemicals) along with any new data which you may need to add to the Chemical Database, and
- (3) a draft of a list of reactions.

Information

Fill in the UDL File Name (you don't need to add the .UDL extension), lab Title and lab Description, then select Next. This information will appear in the Simulation Module dialogue box.

Author is optional. (Note that you may include your e-mail address here.)

Password protection is available in order to prevent unwanted tampering with lab module design or viewing of information such as the names of unknown chemicals and other lab details.



documentation

Specify your Introduction, Procedure and Observations file locations (no need to provide extensions), then select Next.

If you haven't already created these documents, you may use any wordprocessor that can save in Rich Text Format (i.e. *.rtf). Note you must copy your RTF(s) to the ChemLab folder for inclusion in the UDL file. Once created, these files will be displayed in separate windows for your users on the left-hand side of Chemlab's environment. In the Introduction document you should include the reasons for conducting the experiment and the theory behind it, including the formulas for the reactions to be performed. In the Procedure document you should include the step-by-step instructions for conducting the experiment, making special note of the quantities of chemicals required. The Observation document should be formatted such that the items to be observed are listed on the left-hand side and blank spaces are provided on the right-hand side. Users may then record observations and required calculations directly in ChemLab. Upon completion of the lab, users may save their results to a file, either on disk or on a network file server. If the lab is used as part of a student's course work, observations in the form of a lab file may be submitted for grading.

If you are editing a UDL provided to you without these files, the Lab Wizard will use the documentation information already stored in the UDL file.



chemicals

Before you create your customized lab module, you must check to make sure that all the chemicals required for your products, reactants, and all intermediate reactions used in the process are available in the Chemicals Database. If they are not, don't panic. You can always add to the database yourself. (Note that water is automatically included in the Added Chemicals list.)

Use the Chemical Database scroll bar to search for each of the chemicals on your required chemicals list. If you find one, select << ADD and check it off your list. If you've added something you don't need in your lab, select Remove>> to delete it from the Added Chemicals list. Once a chemical has been imported from the database, its properties must be specified in the Chemical Properties dialog box. It appears automatically when a chemical is dropped, but may also be accessed by highlighting a chemical and selecting the Chemical Properties button.

If new chemicals need to be added to the Chemical Database, select Add new chemicals to database

If you need to change the specifications for a new chemical you've added to the database, you may highlight the chemical in the database column and select Edit chemical database.



chemicals database

The Chemical Database services as a repository for chemical data for use in UDL labs.

The following are the properties listed for each new chemical in ChemLab's Chemical Database:

Name:
Formula:
Description:
GMW: _____ (required for all chemicals)
Density: _____ g/cm³ (optional for ions)
Boiling Point: _____ C (optional for ions)
Melting Point: _____ C (optional for ions)
Color: _____ (see color dialog box)
Fill Pattern: _____ (used to indicate crystal, powder, or sold)
Heat Capacity: _____ J/Mol K (at constant pressure)
Ion Charge: _____ (e.g. -1 or +2)
State: _____ (Solid, Liquid, Gas, or Ion)
Solubility in Water
 at 0 C : _____
 at 100 C : _____

CAS RN: _____ - _____ - _____ (CAS registry number)



Chemlab uses solubility to determine how much of a substance is in solution. Ions are produced by the dissociation of a compound in solution. For example, HCl becomes H⁺ and Cl⁻ in solution. If ions are required for intermediate reactions, then they must be added to your chemical list from the database.



The following web sites may be helpful for chemical research:

<http://chemfinder.camsoft.com>
<http://www.krinfo.ch/krinfo/products/datastar/sheets/CSEM.HTM>
<http://www.chem.ucla.edu/chempointers.html>

chemicals properties dialogbox

The Chemical Properties dialog box appears when adding a chemical to the Chemicals List from the Chemical Database. Of particular importance is classifying each chemical as either a Stock Chemical, a Reaction Product, a Unknown, or a Solution. Some of these properties are exclusive. A Reaction Product cannot also be a Solution. Solutions are prepared according to the specified molarity (e.g. 1 M HCl) and, along with Stock Chemicals, are provided to the ChemLab user in the available chemicals list in the Chemicals dialog box. Since Reaction Products are produced by a reaction, they are not available to the user and do not appear in the chemicals list. An Unknown chemical is a reactant to be solved for by the user. The name specified under Unknown Name appears in the available chemical list in place of the chemical's actual name.



reactions

The formulas for your chemical reactions are entered into the UDL by means of a reaction tree. Before using the Lab Wizard, you may want to draw a reaction tree for your experiment. The structure of the tree is the same as the familiar structure of file directories or folders found on a disk. The root directory is always Reactions. From here you must create separate sub-directories for each reaction, which in turn contain separate sub-directories for Reactants and Products.

The order of reactions moving down the tree is the order in which reactions will be simulated by ChemLab's stoichiometry reaction engine. All dissociation reactions should be executed first. Some reactions will have precedence over other reactions. Hence, it's possible that one reaction may consume all the chemicals for another reaction before it begins, preventing it from occurring at all.

Start adding reactions by selecting the Add Reaction button. A Reaction Detail dialog box will appear. A new entry will appear in the Reaction Tree. Drag and drop chemicals from the available Chemical List to the leaf nodes labeled Reactants and Products. The "NO" symbol, the circle with the slash through it, indicates where chemicals may not be dropped.

Once reaction tree nodes are in place reactions may easily be manipulated by highlighting a particular reaction node and selecting one of the available button options. Button options include: Edit Reaction, Delete Reaction, Move Up, or Move Down.

Once chemicals have been dropped they may easily be edited or deleted by highlighting a particular reactant or product and selecting one of the available button options.

Clicking on a reaction node displays the chemical formula for the reaction along with the mass balance for the left-hand side (LHS) and the right-hand side (RHS) of the equation. Looking to see whether or not the LHS and RHS values are equal is a quick way to check that the formula was entered correctly.



reaction detail

Name reaction and set any reaction conditions.

Reaction Rates maybe set as instantaneous, fixed, or varying with concentration.

Instantaneous is self-explanatory. Fixed rate means that the reaction occurs at the rate the first reactant is consumed in mole/L(sec). Setting this rate simulates a reaction occurring over a period of time. For a reaction that varies with concentration, the rate of reaction may set to depend upon the concentration of reactants. Given the reaction:



The reaction rate is expressed as the rate of change of the concentration of the first reactant. The relationship that exists may be expressed as:

$$\text{rate} = d[A]/dt = k([A]^m[B]^n)$$

or rate of change of the concentration of X

where K = rate constant, (units are M/s)

m = order of the reaction with respects to the concentration of A

n = order of the reaction with respects to the concentration of B

ChemLab only allows for the rate to be affected by the concentration of the first two reactants only. The positioning of chemicals when adding a reaction is therefore important.



reaction chemical

The Reaction Chemical dialog box appears when you drag a chemical from the Available Chemicals list and drop it as a reactant or product. It is used to enter the coefficient for the chemical and assign attributes that affect the appearance and use of the chemical in the reaction.

(1)The "Precipitate" check box indicates that a product is shown as a solid precipitate when formed.

(2)The "Must be in solution" check box indicates that a reactant which is a solid must be dissolved into a solution before it is used in the reaction. This is typical of dissociation reactions of the form $AX(aq) \rightarrow A^- + X^+$.

(3) The "Solution Color Changes" option is used to cause a change in the color of a solution to indicate that this chemical has been produced. The change option is set by selecting the "Causes color change in solution" check box. The color of the solution will change instantaneously to whatever color has been selected on the left-hand side when the chemical reaches the molar concentration entered on the right-hand side. If you wish the color change to be gradual, you must select the "Use color range" checkbox. The color of the solution will change gradually over the range of colors specified on the left-hand side as the concentration of the chemical increases or decreases as specified on the right-hand side. Note that only one color change will be shown by ChemLab. Hence, you should only mark one product in a reaction to change solution color. If a number of reactions are set to cause a color change, only the color change for the last active reaction will appear.



password

Password usage is optional. It's a good idea if you want to prevent your students hacking into the lab module. However, if you plan to distribute this UDL, you will have to send the password along with it. Otherwise, it will be useless to others. Note that you can remove password protection by deselecting the check and re-entering the password.



