USER MANUAL – TEST: #0054

DEVELOPED BY SAMUEL MCKID

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INSTALLATION

Downloading

The program can be found on GitHub, at: https://github.com/MCSQU1D/Test_-0054/releases. Click on the latest version, and download the compressed source code.

Setting up

This program runs on python, so you must install python on your computer. The instructions to install can be found here: https://www.python.org/downloads/. The recommended version is 3.7.6 found here: https://www.python.org/downloads/release/python-376/.

Inorder for the program to work, you must install the pygame library. Instructions to install this library can be found here: https://www.pygame.org/wiki/GettingStarted. The recommended version is 2.0.14.

Ensure that the directory is uncompressed and on your computer desktop.

STARTING AND SETTING UP

Launching Application

The program can be run with the following command entered into the command line (you may need to change the “3.0” to suit your version):

```
cd Desktop/Test_-0054-3.0
```

Followed by:

```
python3 FileA.py
```

The program will launch into the start screen.

Legal Information and Agreements

All legal information regarding the installation and operation of the “Test: #0054” chemical simulator can be found in the ‘legal’ tab at the bottom left of the launch screen. A single click will open this tab (figure I), and a single click on the same location will close the tab (figure II). For your convenience, a copy has been attached below, but may be subject to change without notice.

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Legal Information and Disclaimer

Do NOT attempt to recreate any experiments possible in this simulator. Any attempt to recreate experiments may result in damage to property and serious injury or death. Sam McKid, or other individuals or organisations involved within the development of this program, are NOT liable for any damage to property or individuals as a result of attempted recreation. The recreation of any experiments displayed in this simulator may breach laws and regulations. Check your local authorities for more information. While all attempts have been made to ensure the accuracy of the information, this simulator is NOT a reliable source of information. The simulated reactions/ experiments are NOT approved for academic study. Do not modify any files within the program. Do not distribute modified versions of this program. Distribution of original/unmodified versions may be permitted with explicit authorisation from developer(s).

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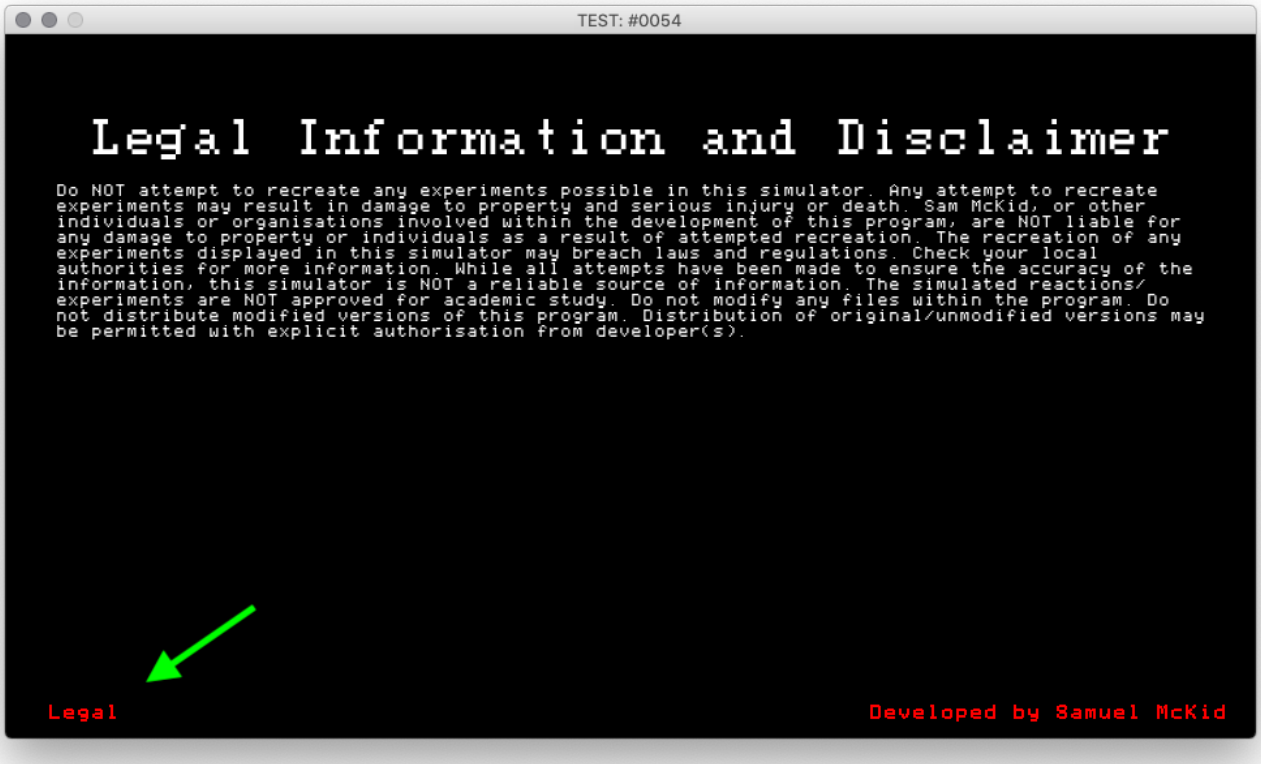
Figure I


TEST: #0054
TEST:#0054
the premier chemical stimulator
BEGIN
QUIT
Legal
Developed by Samuel McKid

Figure II


TEST: #0054
Legal Information and Disclaimer
Do NOT attempt to recreate any experiments possible in this simulator. Any attempt to recreate experiments may result in damage to property and serious injury or death. Sam McKid, or other individuals or organisations involved within the development of this program, are NOT liable for any damage to property or individuals as a result of attempted recreation. The recreation of any experiments displayed in this simulator may breach laws and regulations. Check your local authorities for more information. While all attempts have been made to ensure the accuracy of the information, this simulator is NOT a reliable source of information. The simulated reactions/ experiments are NOT approved for academic study. Do not modify any files within the program. Do not distribute modified versions of this program. Distribution of original/unmodified versions may be permitted with explicit authorisation from developer(s).
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BASIC FUNCTIONALITY

Simulator Screen Controls

The simulator screen (figure III) is a black screen with various buttons and rectangles. The large central rectangle is the workspace, where all reactions will take place. The bottom rectangle is an information panel that will describe what the cursor is hovering over. On the right are the molecules and controls.

Figure III

Workspace
Within the workspace, there are 4 information displays (from top left to right): frames per second (FPS), particle count, temperature, and the coordinates of the mouse cursor. The coordinates of the mouse cursor will disappear when the mouse is out of the workspace. The cursor will also be replaced by a small square, indicating the area in which molecules are placed (only when the cursor is in the workspace).

Information Panel
This panel at the bottom of the screen will describe what the cursor is hovering over, and any keyboard shortcuts available.

Molecule Buttons
On the right hand side of the screen are the molecules at the top right, and the controls at the bottom right. The molecules are labeled by the chemical symbol, and will display the colour of each molecule when selected (as seen with helium in figure IV). Clicking on the molecule button will equip it to be placed in the workspace.

Control Buttons

The controls at the bottom right are:

- INF (display molecule information menu, can use ‘i’ key)
- PSE (Play/pause the simulation, can use spacebar)
- CLR (Clear the simulation, can use ‘c’ key)
- ↑ (Increase temperature, can use up arrow and left shift to boost)
- ↓ (Increase temperature, can use down arrow and left shift to boost)

When the molecule information menu is showing or the simulator is paused, the ‘INF’ and ‘PSE’ buttons will glow white respectively (seen in figure IV, both are activated)

Molecule Information Menu

The molecule information menu will be shown in the left third of the workspace, and displays information regarding the selected molecule (seen for Helium in figure IV)

Figure IV

Mouse Controls

Hovering the cursor over an area will display the function on the information panel.

Left clicking on buttons will select the molecule or do the control function. Left clicking on the workspace will place the selected molecule in the area of the cursor. Be careful not to hold the click down for long as excessive molecules may be added, causing large amounts of lag.

Right clicking on molecules within the workspace will remove these molecules.

Keyboard shortcuts

The simulator is primarily operated by mouse clicks, although there are several keyboard shortcuts. These are;

- ‘i’, display molecule information menu
- ‘c’, clear the workspace of molecules
- spacebar, pause the simulator
- up arrow, increase screen temperature
- down arrow, decrease screen temperature
- left shift, boost the temperature change of up arrow and down arrow

Selecting Molecule

To select a molecule, left click on one of the molecule buttons on the top right of the screen. The button will change to the colour of the molecule if selected. This can be seen in figure V, where hydrogen ‘H’ is selected, and has changed to the blue shade of the hydrogen molecule. When another molecule is selected, the first molecule button will change back to the black button with white background.

Figure V

Molecule Information Menu

When a molecule is selected, clicking on the ‘INF’ button will display the information menu as will pressing the ‘i’ key. In Figure VI, Hydrogen ‘H’ is selected, and the information menu is displayed. The ‘INF’ button will invert colours, either if it was clicked or the ‘i’ key was pressed. The menu will display various points of information about the molecule, and has a diagram of the atomic structure for elements (‘H’ to ‘Au’) or the chemical structure of compounds (‘H2O’ to ‘AlO’).

Figure VI

Placing and Removing Molecules

Once a molecule has been selected, left clicking on the workspace will place molecules. The cursor ‘square’ will be filled with molecules when placed, and will continue to place molecules in the same place while the click is held down. Therefore, care should be taken in placing molecules as a large amount can be placed in very little time, causing a large amount of lag.

To remove a molecule, right click with the target molecules within the cursor ‘square’. All molecules within the square will be removed. Alternatively, pressing the ‘CLR’ button or the ‘c’ key will remove all molecules.

ADVANCED FUNCTIONALITY

Starting Reactions

Reactions will occur when the reacting molecule(s) are within proximity of each other, and a certain temperature has been reached. These molecule(s) will react, replacing the reacting molecule(s) and forming the resultant molecule(s). The reaction will have an effect on the temperature of the screen.

Reactions possible:

Reacting Molecule(s)	Resulting Molecule(s)	Temperature Required	Temperature Added
Hydrogen (‘H’) Oxygen (‘O’)	Water (‘H2O’)	500°C	500°C
Iron (‘Fe’) Oxygen (‘O’)	Iron Oxide (‘FeO’)	-273.15°C	0°C
Aluminium (‘Al’) Oxygen (‘O’)	Aluminium Oxide	-273.15°C	0°C
Iron Oxide (‘FeO’) Aluminium (‘Al’)	Iron (‘Fe’) Aluminium Oxide	900°C	4000°C

Temperature

The temperature of the screen is displayed in the top middle of the workspace, however there are other temperatures in the simulator. Each molecule will have an individualised temperature, which will slowly adjust to the screen temperature. However, the screen temperature will also adjust to the average temperature of the molecules. This means that continuous reactions will occur (i.e. reactions that require the heat produced by previous reactions).

Controlling temperature

Temperature is increased or decreased by the ‘↑’ or ‘↓’ buttons respectively. The up arrow and down arrow will also increase/decrease the temperature, with the shift key to boost the rate of change. The up arrow will change the temperature at 60°C/second, whereas the shift key will boost this to 6060°C/second. The ‘↑’ and ‘↓’ buttons allow for precise adjustment.

Custom Molecules and Reactions

While more advanced than previous functions, creating/modifying molecules and reactions is still relatively easy to do. Firstly, you must navigate to the “Test_-0054” directory. From there navigate to the “files” directory. Within the “files” directory, there are 2 .txt files, “chemicalinfomation.txt” and “chemicalreaction.txt”.

Custom Molecules

The .txt file (chemicalinfomation.txt) is organised in the following pattern:

Chemical Name|Chemical Symbol/Formula|Protons/Composition|Atomic Mass|State at room temp|Melting Temp|Boiling Temp|Information|R|G|B

This can be found at the top of the file (DO NOT DELETE). Below (each on a new line), you will find the molecules in the program in the same format. To create a new molecule, simply copy the top line (the one shown above), and fill in the values. Do not leave spaces on any numerical values or on in the symbol/formula part, and be careful not to create a new ‘empty’ line below the last molecule. A 180x180 .jpg image can be place in the ‘file’ directory with the filename of the molecule name followed by “_structure.jpg”

NOTE: Temperature values are in Celcius.

Custom Reactions

The .txt file (chemicalreaction.txt) is organised in the following pattern:

Reactant_1|Reactant_2|Result|Temp required|Temp result

This can be found at the top of the file (DO NOT DELETE). Below (each on a new line), you will find the reactions in the program in the same format. To create a new molecule, simply copy the top line (the one shown above), and fill in the values. Do not leave spaces on any numerical values or on in the symbol/formula part, and be careful not to create a new ‘empty’ line below the last molecule. Using a “+” between result molecules will create 2 different molecules (i.e. FeO will create an Iron Oxide molecule, Fe+O will create Iron molecule and Oxygen molecule).

NOTE: Temperature values are in Celcius.

TROUBLESHOOTING

Problem	Possible Solutions
Program won't start	Make sure you entered the commands correctly in order (see Launching Application) Make sure all files and directories are uncompressed and in correct location (see Downloading and Setting up) Quit command line/terminal and restart the process (see Launching Application) Make sure all edits to .txt files are correct (see Custom Molecules and Reactions)
I can't place molecules	Make sure a molecule is selected (see Selecting Molecule)
I place particles but nothing happens	Make sure that the simulator is not paused (see Control Buttons under Simulator Screen Controls)
Reactions aren't happening	Make sure the right molecules are within proximity (see Starting Reactions) Make sure temperature is sufficient (see Starting Reactions)
The simulator is too laggy	Remove particles by right clicking with square cursor (see Placing and Removing Molecules) or by pressing the 'CLR' button or the 'c' key (see Simulator Screen Controls)