Flash Separator Simulator - Instruction Document

This document is a user manual designed to accompany the Flash Separator Simulator.

1) Starting & Running the Program

To start the program, the *MainClass.java* file must be opened in a suitable java Integrated Development Environment (IDE). The *MainClass.java* file may be found within the *flashseparator* folder.

> DrJava, Eclipse and NetBeans are examples of suitable IDEs.
> Instructional figures in this document were created using DrJava.

Once the file is open in the IDE, the program may be compiled & ran. The user interface for the program is provided via the console.

Warning: *For some versions of DrJava, the simulation program will only run if all of the class files are opened upon the first time running the program (but will run in future with only the MainClass.java file out). If there the user encounters issues compiling/running with only the MainClass.java file open, open all of the other files in folders* ***eos****,* ***fileimport****,* ***flashseparator*** *&* ***numericmethods****. Then re-try compiling and running the program.*

Upon running, the user will be prompted to select one of two options, which are to be selected by entering a letter. The available options and its corresponding letter are shown below.

Option	Letter entry	Description
Instructions	i	Provides basic program instructions to the user
Run Simulation	r	Runs the simulation, using the information in the input CSV files.

Before running the simulation, the user must ensure that the input files have been created for the simulation. Input and Output is managed by an accompanying Excel File, "*Flash Simulation IO Form*". Refer to the next section for instructions on how to create the required CSV files using the Excel document.

Once the required CSV files have been created, the program can be run. At program start-up, the Main Menu appears as follows:

```
CHG4343 - Flash Separation Simulator

Welcome to the flash separation simulator. Please enter a letter corresponding to one of the following options:
Enter "i" for instructions on how to use this program.
Enter "r" to run a simulation.
```

Details pertaining to both options are presented below.

(i) Instructions

The instructions included within the program simply specify the purpose of the program and what types of simulations it is designed to perform.

```
Instructions

This program allows users to simulate a flash separation process for three different cases. In each case the tank pressure, feed composition, feed flowrate and a temperature must be
specified. These inputs are used to calculate the vapour and liquid product compositions and flowrates, as well as a third parameter. The third parameter calculated depends on the
user-specified temperature. The three possible cases are described below:

      Case 1 - Specified: constant operating temperature, Determined: heat to maintain the operating temperature.
      Case 2 - Specified: feed temperature, Determined: flash temperature.
      Case 3 - Specified: flash temperature, Determined: feed temperature.

In addition to the specified parameters, species properties for the species in the inlet stream must also be specified. This program has an accompanying excel file (Flash Simulation IO
Form), where the species properties and system parameters are specified. This excel file is used to generate .csv files containing all the information needed to run the program. The
program is designed to automatically read these CSV files upon running. Please refer to the excel file for instructions pertaining to its use.

To perform a simulation, complete the excel form & create the CSV files. Once this is complete, the simulation may be run by entering "r" in the welcome menu.
Please enter enter "r" to run the simulation immediately, or enter any other letter/symbol to return to the main menu.
```

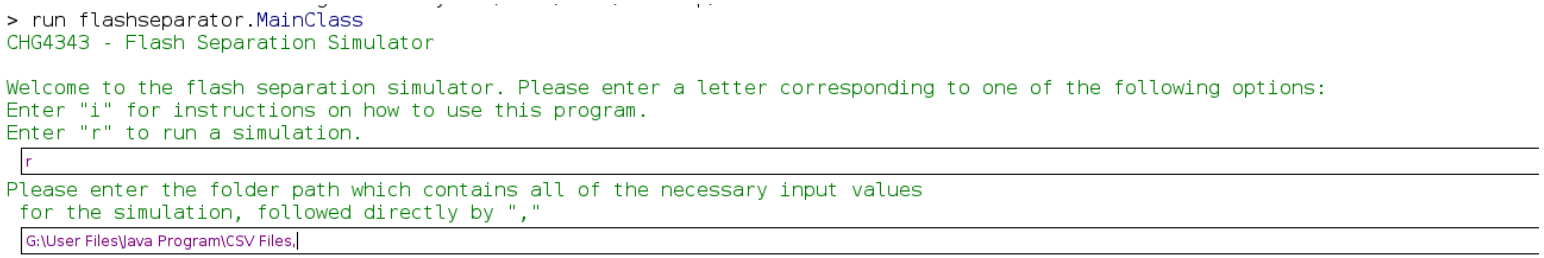
From here, users may run the program, by entering “r” into the console or may return to the main menu by entering any other letter/symbol (ie. “l” or “,”). All inputs into the console are performed through the keyboard.

(ii) Run Simulation

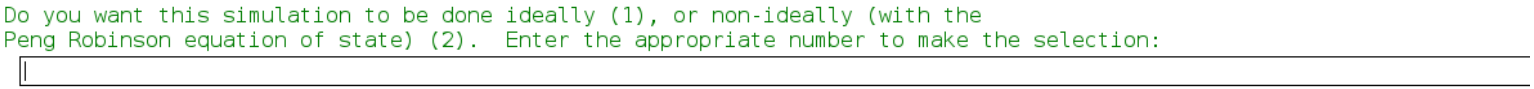
When the program is run, either by entering “r” from the Main Menu or from the Instructions, the user is prompted to enter a folder path.

```
Please enter the folder path which contains all of the necessary input values
 for the simulation, followed directly by ","
```

Copy and paste in the path to the folder containing the CSV files, and then indicate the end of the path with a comma (“,”). *The comma must come directly after the path name (no spaces), otherwise the path will not be read correctly.* An example of an appropriate file path is shown below.



Next, the user will be asked whether they want the simulation to be done based on the assumption of ideality, or non-ideality. The latter is carried out using the Peng Robinson equation of state. To perform a simulation under the assumption of ideal conditions, enter “1”. To perform a simulation under the assumption of non-ideal conditions, enter “2”.



The desired simulation will execute, and the results will be printed to a .csv file (*systemoutput.csv*).

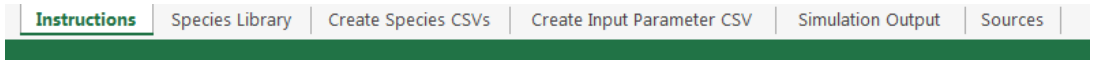
Upon successfully completing the simulation, a statement will print out indicating the location of the outputted CSV file. *This location should be the same as the path previously indicated by the user, containing the input CSV files*. For example, in the case of the example shown above, the following statement would appear:

System output has been saved in G:\User Files\Java Program\CSV Files as systemoutput.csv

The results may be viewed directly from this .csv file, or they may be imported into the *Flash Simulation IO Form*, as described in (ii) Output (in Section 2).

2) Input/Output management: Flash Simulation IO Form

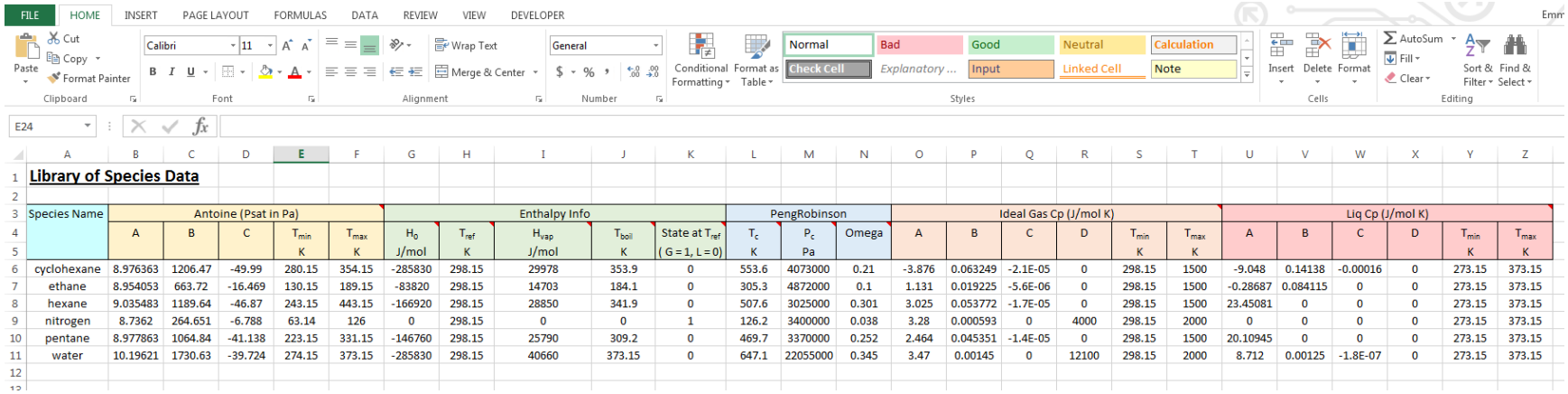
The *Flash Simulation IO Form* is a macro-enabled Excel document (.xlsm) designed to handle IO for the Flash Separator Simulator. It has six tabs, as shown below:



Basic instructions on how to use the form are included in the “Instructions” tab. More detailed instructions are included here, broken up into (i) Input and (ii) Output.

(i) Input

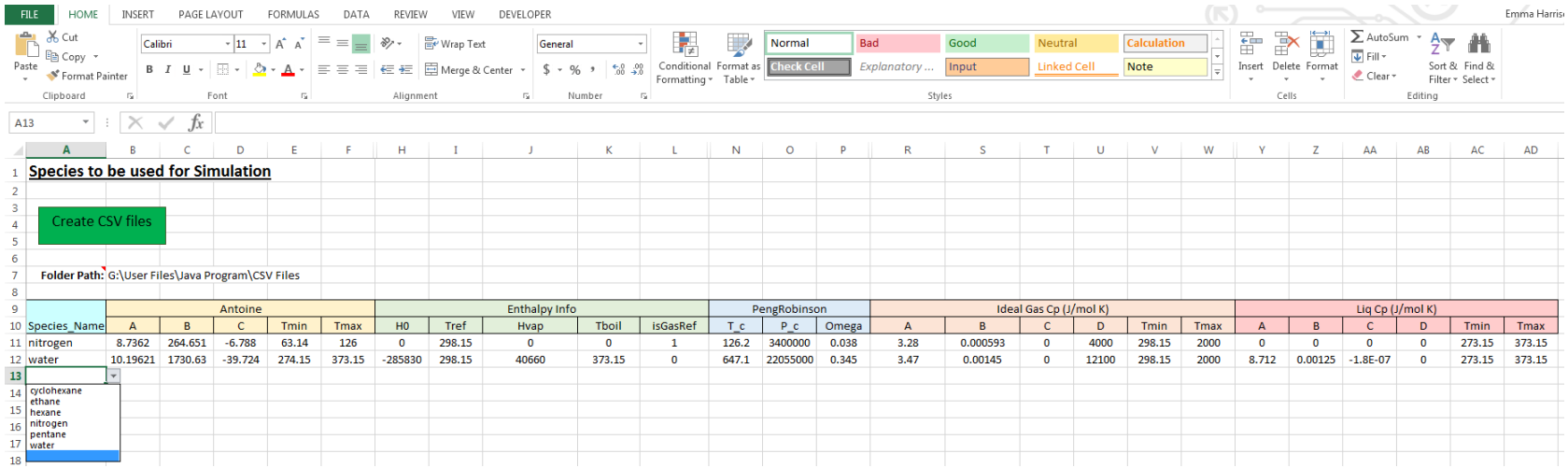
Two types of input files must be created for the simulation: chemical species properties & system parameters. Chemical species properties that are needed for the simulation are stored in the “Species Library” tab, as shown in the figure below.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
1	**Library of Species Data**																									
2																										
3	Species Name	Antoine (Psat in Pa)					Enthalpy Info					PengRobinson			Ideal Gas Cp (J/mol K)						Liq Cp (J/mol K)					
4		A	B	C	T_{min}	T_{max}	H_0	T_{ref}	H_{vap}	T_{boil}	State at T_{ref}	T_c	P_c	Omega	A	B	C	D	T_{min}	T_{max}	A	B	C	D	T_{min}	T_{max}
5					K	K	J/mol	K	J/mol	K	(G = 1, L = 0)	K	Pa						K	K					K	K
6	cyclohexane	8.976363	1206.47	-49.99	280.15	354.15	-285830	298.15	29978	353.9	0	553.6	4073000	0.21	-3.876	0.063249	-2.1E-05	0	298.15	1500	-9.048	0.14138	-0.00016	0	273.15	373.15
7	ethane	8.954053	663.72	-16.469	130.15	189.15	-83820	298.15	14703	184.1	0	305.3	4872000	0.1	1.131	0.019225	-5.6E-06	0	298.15	1500	-0.28687	0.084115	0	0	273.15	373.15
8	hexane	9.035483	1189.64	-46.87	243.15	443.15	-166920	298.15	28850	341.9	0	507.6	3025000	0.301	3.025	0.053772	-1.7E-05	0	298.15	1500	23.45081	0	0	0	273.15	373.15
9	nitrogen	8.7362	264.651	-6.788	63.14	126	0	298.15	0	0	1	126.2	3400000	0.038	3.28	0.000593	0	4000	298.15	2000	0	0	0	0	273.15	373.15
10	pentane	8.977863	1064.84	-41.138	223.15	331.15	-146760	298.15	25790	309.2	0	469.7	3370000	0.252	2.464	0.045351	-1.4E-05	0	298.15	1500	20.10945	0	0	0	273.15	373.15
11	water	10.19621	1730.63	-39.724	274.15	373.15	-285830	298.15	40660	373.15	0	647.1	22055000	0.345	3.47	0.00145	0	12100	298.15	2000	8.712	0.00125	-1.8E-07	0	273.15	373.15
12																										

Currently, only species information for the six species required for the project (cyclohexane, ethane, hexane, nitrogen, pentane & water) are specified. If simulations with other species are desired, their information will need to be added to the library.

The CSV files containing the necessary species properties are created under the “Create Species CSVs” tab. Information for this sheet is populated using the species information stored in the *Species Library*. To include a given chemical species for a simulation, simply select it from the drop down menu under “Species_Name”. Its information will be automatically populated by the information stored in the library.



Species to be used for Simulation

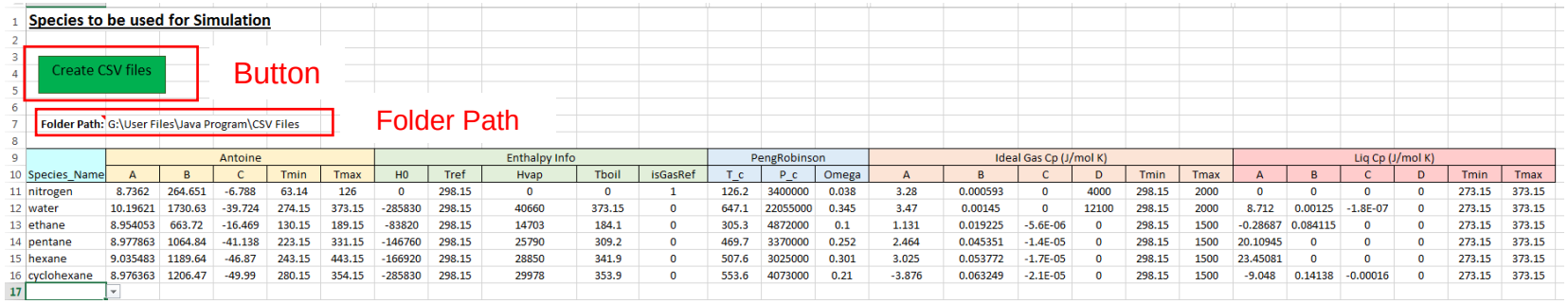
Create CSV files

Folder Path: G:\User Files\Java Program\CSV Files

	Antoine					Enthalpy Info					PengRobinson			Ideal Gas Cp (J/mol K)						Liq Cp (J/mol K)					
Species_Name	A	B	C	Tmin	Tmax	H0	Tref	Hvap	Tboil	isGasRef	T_c	P_c	Omega	A	B	C	D	Tmin	Tmax	A	B	C	D	Tmin	Tmax
nitrogen	8.7362	264.651	-6.788	63.14	126	0	298.15	0	0	1	126.2	3400000	0.038	3.28	0.000593	0	4000	298.15	2000	0	0	0	0	273.15	373.15
water	10.19621	1730.63	-39.724	274.15	373.15	-285830	298.15	40660	373.15	0	647.1	22055000	0.345	3.47	0.00145	0	12100	298.15	2000	8.712	0.00125	-1.8E-07	0	273.15	373.15

cyclohexane
ethane
hexane
nitrogen
pentane
water

Once the desired chemical species have been included, the species properties CSV files are created by clicking the “Create CSV Files” button. Before generating the CSV files, please ensure that the correct Folder Path is indicated. The folder path can be anywhere the user desires, however all input and output CSV files should come from/go to the same location (since this same folder path will be entered when running the simulation).



Species to be used for Simulation

Create CSV files — Button

Folder Path: G:\User Files\Java Program\CSV Files — Folder Path

	Antoine					Enthalpy Info					PengRobinson			Ideal Gas Cp (J/mol K)						Liq Cp (J/mol K)					
Species_Name	A	B	C	Tmin	Tmax	H0	Tref	Hvap	Tboil	isGasRef	T_c	P_c	Omega	A	B	C	D	Tmin	Tmax	A	B	C	D	Tmin	Tmax
nitrogen	8.7362	264.651	-6.788	63.14	126	0	298.15	0	0	1	126.2	3400000	0.038	3.28	0.000593	0	4000	298.15	2000	0	0	0	0	273.15	373.15
water	10.19621	1730.63	-39.724	274.15	373.15	-285830	298.15	40660	373.15	0	647.1	22055000	0.345	3.47	0.00145	0	12100	298.15	2000	8.712	0.00125	-1.8E-07	0	273.15	373.15
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pentane	8.977863	1064.84	-41.138	223.15	331.15	-146760	298.15	25790	309.2	0	469.7	3370000	0.252	2.464	0.045351	-1.4E-05	0	298.15	1500	20.10945	0	0	0	273.15	373.15
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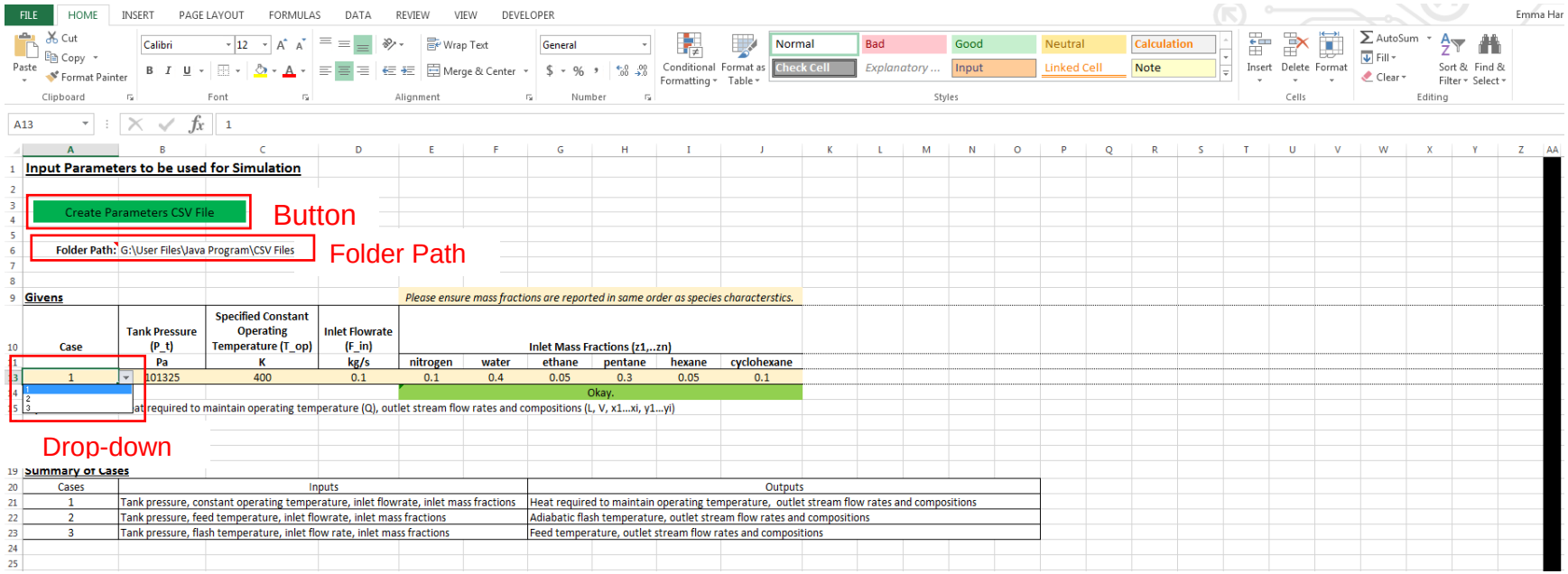
cyclohexane	8.976363	1206.47	-49.99	280.15	354.15	-285830	298.15	29978	353.9	0	553.6	4073000	0.21	-3.876	0.063249	-2.1E-05	0	298.15	1500	-9.048	0.14138	-0.00016	0	273.15	373.15

The following five CSV files will be output to the indicated folder location: *antoine.csv, enthalpy.csv, gasCp.csv, liqCp.csv, pengRobinson.csv*.

Next, the system parameters CSV file can be created from the “Create Input Parameter CSV” tab. The system parameters required for the simulation depend on the case being executed. The case is selected from the drop-down menu under “Case” (under Givens). The required givens are updated based on the case, the user must provide the information specified. A summary of the three possible cases is provided at the bottom of the sheet.



Once the case is selected and the necessary information filled out, click the “Create Parameters CSV File” button to create the following CSV file: *caseParameters.csv*. Note once again, that the output path must be specified. This should be the same path as the one used for outputting the CSV files containing the species properties.

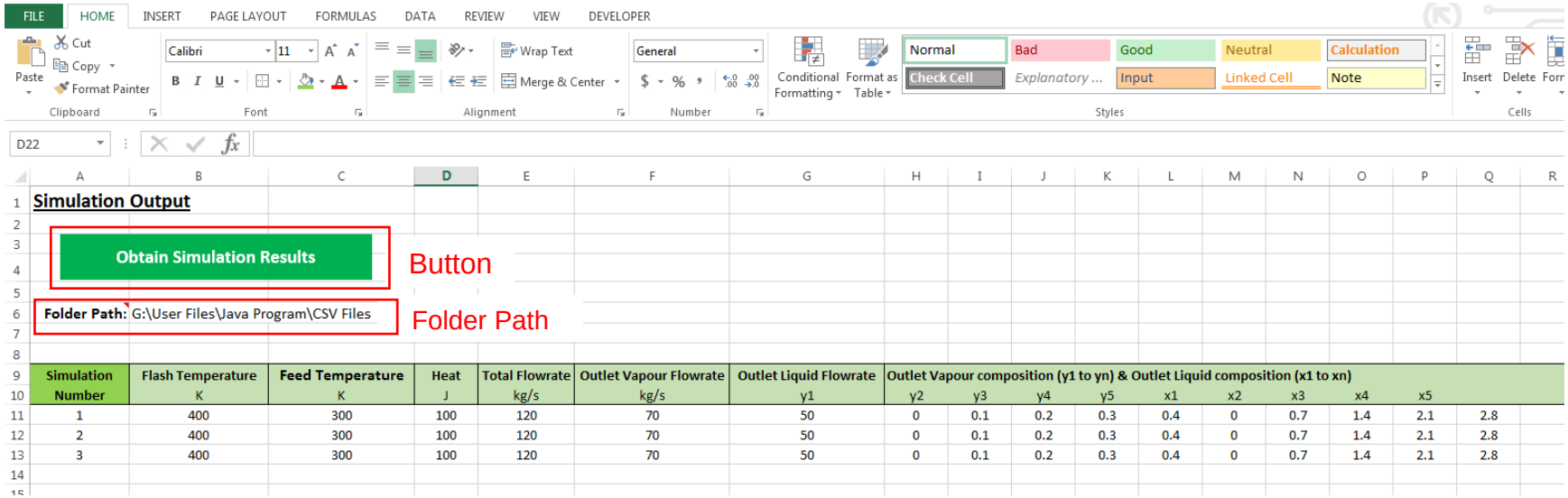
Warning: *the values for the parameters don’t change when the case is changed, therefore when the case is changed, the parameters will still be filled out with the previous case’s values, and must be updated manually for the new case.*

Once these seven CSV files have been created. The simulation can be run, by entering “r” from the program start up menu (as described in Section 1: Starting the program).

(ii) Output

When the simulation is complete, it automatically outputs the data within a CSV file (*systemoutput.csv*) to the folder indicated upon running the program (folder where the input CSV files are located). Users may use the data from this file directly, or may import it into the *Flash Simulation IO Form*. For the latter, the “Simulation Output” tab is set up to import the data from the CSV file, with the click of a button.

Once the simulation has been run (and the *systemoutput.csv* file created), navigate to the “Simulation Output tab”, ensure that the indicated Folder Path is correct, and click “Obtain Simulation Results”. The results will appear on the next blank line. Lines containing data may be deleted & re-populated as desired. This allows for easy comparison between simulations performed with different conditions.



Simulation Number	Flash Temperature K	Feed Temperature K	Heat J	Total Flowrate kg/s	Outlet Vapour Flowrate kg/s	Outlet Liquid Flowrate y1	Outlet Vapour composition (y1 to yn) & Outlet Liquid composition (x1 to xn) y2	y3	y4	y5	x1	x2	x3	x4	x5
1	400	300	100	120	70	50	0	0.1	0.2	0.3	0.4	0	0.7	1.4	2.1	2.8
2	400	300	100	120	70	50	0	0.1	0.2	0.3	0.4	0	0.7	1.4	2.1	2.8
3	400	300	100	120	70	50	0	0.1	0.2	0.3	0.4	0	0.7	1.4	2.1	2.8

The far left column “Simulation Number” is a manual input column. Its purpose is to allow users to keep track of the simulations performed. A number can be specified, or instead details pertaining to each simulation may be entered.