# FLASH SIMULATOR USER GUIDE

## Overview

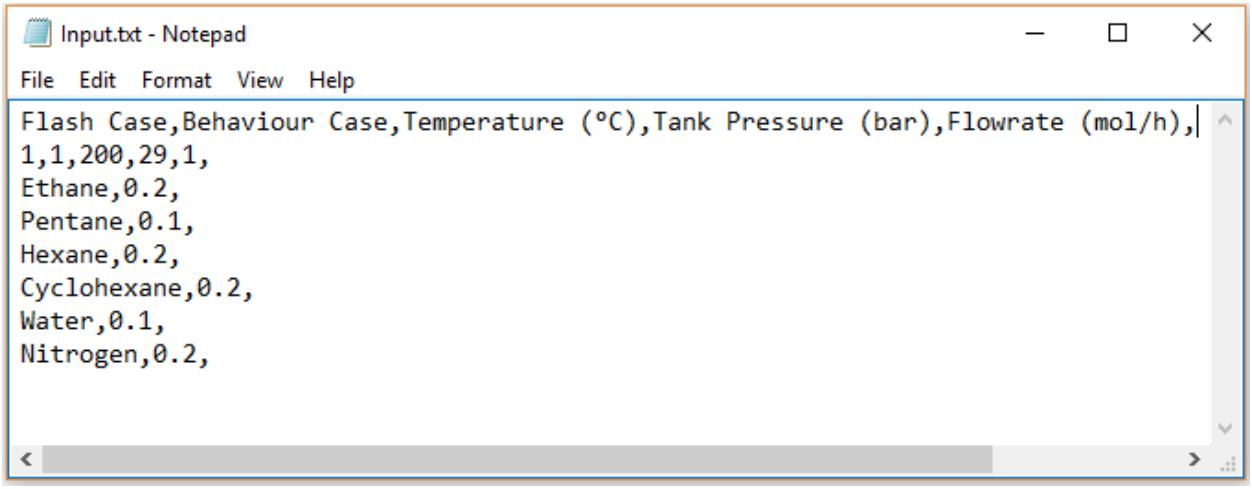
This simulator can be used for flash separation calculations for the following three scenarios:

1. Find the outlet stream compositions, flow rates, and the heat duty required for an isothermal flash.
2. Find the outlet stream compositions, flow rates, and the flash temperature for an adiabatic flash.
3. Find the outlet stream compositions, flow rates, and the feed temperature for an adiabatic flash.

The simulator is programmed for the flash separation of mixtures containing ethane, pentane, hexane, cyclohexane, water, and nitrogen. More chemical species may be added as described later in the user guide.

## Running the Simulator

1. Extract the compressed folder "Code_GROUP22.zip" to the desired computer directory.
2. Open the 34 files with the .java extension in a Java programming environment such as DrJava.
3. Click on the "IO" folder and open the file entitled "Input.txt".




4. In the second line of the Input file, enter numbers corresponding to the flash case, behaviour case, as well as the temperature, tank pressure, and inlet flow rate.
   - For the flash case value: 0 corresponds to the isothermal flash scenario, 1 corresponds to the unknown adiabatic flash temperature scenario, and 2 corresponds to the unknown adiabatic feed temperature scenario.
   - For the behaviour case value: 0 corresponds to ideal flash behaviour, while 1 corresponds to non-ideal flash behaviour.
5. Beginning in the third line of the Input file, enter a component present in the mixture along with its mole fraction in the feed. Each subsequent component and mole fraction must be entered on a new line.

**Note:** All words and values entered into the "Input.txt" file must be separated with a comma with no extra spaces, tabs, or lines entered in between or afterwards. See screengrab of sample input file for proper formatting.

6. After entering the necessary conditions in the "Input.txt file, save the file.
7. In the Java programming environment, click on the "Menu.java" file, compile the code, and run.
8. If the input file has been read correctly, the user will be prompted to enter an option from a menu. Select "1" to continue the flash simulation.
9. If the simulation is successful, results will be sent to the "Output.txt" file which can be found in the "IO" folder. If the flash separation is not possible with the inputted parameters, a message will be printed to the screen.
10. To simulate a flash separation with different parameters, make the necessary changes in the "Input.txt" and save the file. Recompile and run the code.

## Adding a New Chemical Species

- Adding a new chemical species to the flash simulator requires changes to the information in the "Species.csv", "InteractionParameters.csv", and "SubGroups.csv" files in the "IO" folder.
- Open the "Data.xlsx" file.
- In the "Species" tab of the "Data.xlsx" file, each species added will occupy a new row. Add the data required for the component based on the title of each column.
    - Columns 3-10 correspond to some basic chemical and physical property data for the species.
    - Columns 11-18 correspond to the vapour pressure correlation constants and their temperature ranges for the modified Riedel equation of the following form:

      $$P = \exp[A + \frac{B}{T} + ClnT + DT^E]$$

      Where P is in Pa and T is in K. Place a "0" in column 18 for "Form".

    - Columns 19-26 correspond to the liquid heat capacity correlation constants and their temperature ranges.
        - Form 0: $c_{pL} = A + BT + CT^2 + DT^3 + ET^4$
        - Form 1: $c_{pL} = \frac{A^2}{t} + B - 2ACt - ADt^2 - \frac{C^2t^3}{3} - \frac{CDt^4}{2} - \frac{D^2t^5}{5}$

      Where Cp is in J/kmol·K and T is in K.
    - Columns 27-33 correspond to the vapour heat capacity correlation constants and their temperature ranges for the following equation:

      $$\frac{C_p}{R} = A + BT + CT^2 + DT^{-2}$$

      Where T is in K. Place a "0" in column 33 for "Form".

    - Columns 34-37 correspond to the functional groups present in the chemical species for activity coefficient calculations. Place the number of each subgroup present in the chemical species in the appropriate column. If there is a subgroup in the chemical species that is not one of the existing columns, a new column may be added. If a new subgroup is added, ensure a number is placed in the column for each of the species in the file. (Place a "0" in the column is the subgroup is not present in the species).

    - After adding the required components, click “Save As”, choose “CSV (Comma Delimited)” as the file type, and type “Species.csv” as the file name. Ensure the file is saved in the “IO” folder. When prompted whether you would like to replace the existing file, select “yes”. When prompted with a warning that only the active sheet will be saved, select “OK”.
- In the “SubGroups” tab of the “Data.xlsx” file, add the relative volume ($R_k$) and relative surface area ($Q_k$) values for any subgroups which were added to the “Species” tab. These subgroup parameters can be found in Table H.1 of *Introduction to Chemical Engineering Thermodynamics* by Smith et al.
    - After adding the required components, click “Save As”, choose “CSV (Comma Delimited)” as the file type, and type “SubGroups.csv” as the file name. Ensure the file is saved in the “IO” folder. When prompted whether you would like to replace the existing file, select “yes”. When prompted with a warning that only the active sheet will be saved, select “OK”.
- In the “InteractionParameters” tab of the “Data.xlsx” file, add a new column and row for each new subgroup which was added to the “Species” tab. Interaction parameters for other subgroups can be found in Table H.2 of *Introduction to Chemical Engineering Thermodynamics* by Smith et al.
    - After adding the required components, click “Save As”, choose “CSV (Comma Delimited)” as the file type, and type “InteractionParameters.csv” as the file name. Ensure the file is saved in the “IO” folder. When prompted whether you would like to replace the existing file, select “yes”. When prompted with a warning that only the active sheet will be saved, select “OK”.