All modules are now ported to visual basic and the worksheet is updated to conduct all calculations. Please refer to worksheet **PR Solver ver7.**

The code is written in Visual basic that needs to be enabled in Excel to work. Please click allow content when worksheet is opened, follow the below guidelines to open Visual basic.

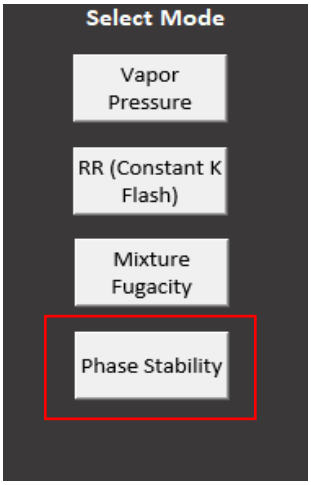
Note: Scripts will not work if macro is disabled in Excel. Ensure you click **Enable Content** when program is opened.

PR Solver ver7

- You can view the visual basic code by turning on developer option in excel
  - Goto file → options → Customize Ribbons → check Developer *in right side tab*
  - Click Developer tab in ribbon (next to View, Review, Data, Home etc)
  - Click Visual Basic
- All static formulas are already built-in different cells.
  - Entire Cardano code is built in cells. For each pressure temperature combo, roots are estimated
  - *Cubic solver is also built in code for programs like fugacity calculation*

- Blue cells mean user input
- Green cells denote calculation results

Selecting Mode



All previous modules that were created in Advanced Thermodynamics course are ported into this worksheet. For Project-2, we are working with **Phase Stability** module. Details of all other modules are provided in the end of this documentation.

Phase Stability & Two-Phase PT Flash

To open the Stability Analysis and Two-Phase PT Flash (SA+Flash) module, click **Phase Stability** from select mode options.

This will take user to SA+Flash worksheet that is used for most parts in Project-2. The main sheet looks like this:

Phase Stability & PT Two Phase Flash | **Isolated Modules** | **Return Home**

Nc	3	Np	2		
Temp (K)	355.372	Pressure	117.2109	R	8.31E-05

Total Z	1

Enter Kij | SA + Flash

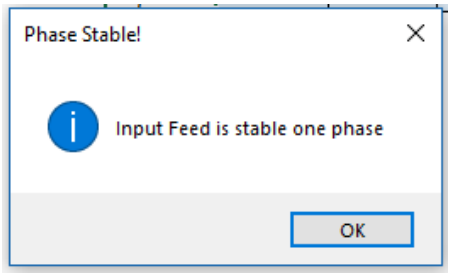
Threshold	1.00E-06	Total Xi	1.000
Max Iteration	1000	Bv	0.441371
PT Flash Iteration	45		
Stability Iteration	132		

Run Phase Stability | Two Phase PT Flash | RR Check | Select Mode

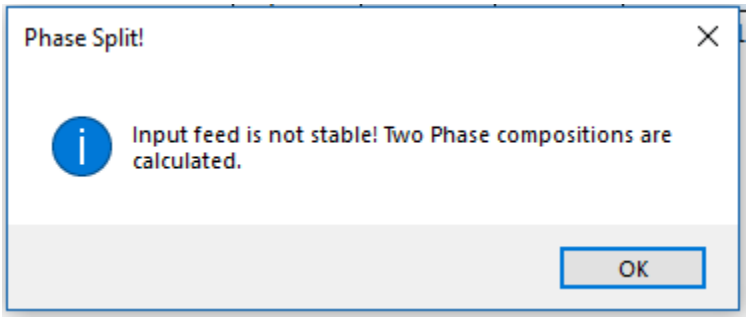
Name	Zi	Tc	Pc	ω	Xi	Yi
CO2	0.8	304.2	73.76494	0.225		
nC4	0.1	425.12	37.96	0.2014		
nC10	0.1	617.7	21.1	0.4898		

Kij Table	CO2	nC4	nC10
CO2		0.12	0.1141
nC4	0.12		
nC10	0.1141		

- All blue cells require user input. User needs to define Nc, Temperature, Pressure, constant R, iteration threshold, max iteration limits and the details of components (overall composition, Critical temperature, Critical Pressure and Acentric Factor)
- After inputting the names of components, click **Enter Kij**. This will create a table for Kij that can be used enter binary interaction parameters
- Once all data is input, click *SA + Flash* to run calculation. This script first conducts stability analysis uses gas-like & vapor-like phase and if either is found unstable, two phase isobaric isothermal flash is conducted to estimate liquid & vapor compositions for each phase. There are three possible outcomes of this calculation:
    1. Entered overall composition (Zi) is stable one phase. The program shows the following prompt.

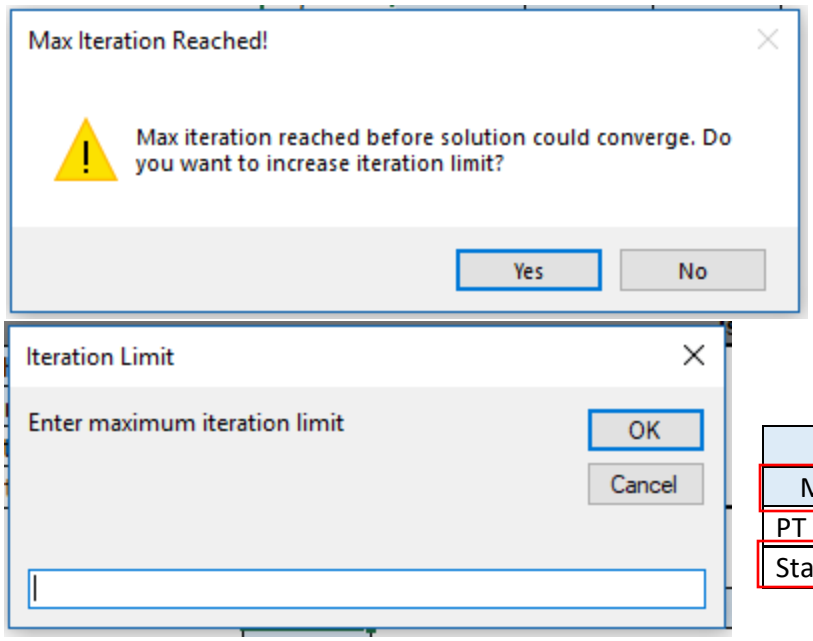


    2. Entered overall composition (Zi) is not stable and is two phase flash is conducted that splits the feed into liquid (Xi) and vapor (Yi) compositions. The program shows the following prompt and phase compositions are shown in table under Green heading Xi and Yi



Xi	Yi
0.710827	0.912863
0.125431	0.067813
0.163742	0.019323

    3. Solution could not converge before the user specified max iteration limit was reached. Same max iteration limit is used for stability analysis and PT Flash. The iteration limit could be reached on either of the sections and will result in similar prompt. User can check whether limit was reached on Stability Analysis or PT Flash by checking the iteration values for each section. Program will prompt user to either increase limit or end run.



Threshold	1.00E-06
Max Iteration	50
PT Flash Iteration	45
Stability Iteration	50

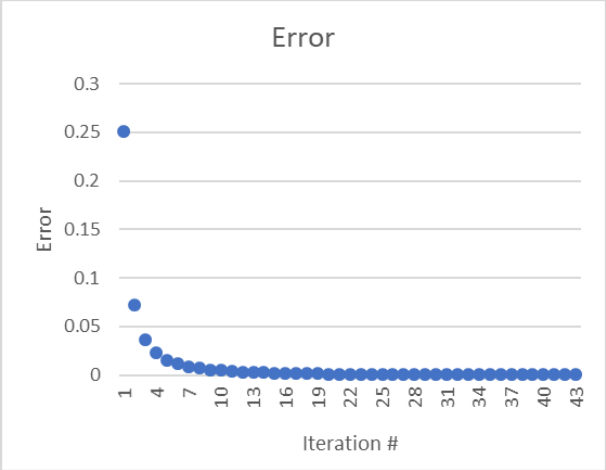
- The total Xi (used to check whether stable or not), Vapor fraction (Bv), iteration used to conduct stability analysis and iteration used to conduct PT Flash are all displayed at end of calculation.

Threshold	1.00E-06	Total Xi	1.000
Max Iteration	500	Bv	0.441371
PT Flash Iteration	45		
Stability Iteration	132		

- As SA+Flash is made up of different isolated modules, they can be run in isolation aswell. In normal operations this is not recommended and is only placed as a tool for quality check and troubleshooting

Isolated Modules			Return Home
Run Phase Stability	Two Phase PT Flash	RR Check	Select Mode

- Error is reduced in each subsequent iteration. This can be checked by the error graph that is plotted at end of each run. Error is plotted for Stability analysis iterations & PT Flash iterations.



Example Calculation

To estimate phase compositions of CO2-nC4-nC10 system at 170 degF (~355 K) and 1700 psia (~117 bar), we follow these steps:

1. Enter Nc, system temperature and pressure and R

Nc	3	Np	2		
Temp (K)	355.372	Pressure	117.2109	R	8.31E-05

2. Enter threshold (1e-6) and max iteration limit (500)

Threshold	1.00E-06
Max Iteration	500

3. Enter details of components

Name	Zi	Tc	Pc	ω
CO2	0.8	304.2	73.76494	0.225
nC4	0.1	425.12	37.96	0.2014
nC10	0.1	617.7	21.1	0.4898

4. Click Enter Kij and input binary interaction parameters

Kij Table	CO2	nC4	nC10
CO2		0.12	0.1141
nC4	0.12		
nC10	0.1141		

5. Click *SA + Flash* to run calculation. As phase is not stable in this case, two phase compositions are calculated.

Name	Zi	Tc	Pc	ω	Xi	Yi
CO2	0.8	304.2	73.76494	0.225	0.710827	0.912863
nC4	0.1	425.12	37.96	0.2014	0.125431	0.067813
nC10	0.1	617.7	21.1	0.4898	0.163742	0.019323