**Documetnation**

1. **Methanation Reactor**
   1. The script “***test1.m***” runs the simulation for the reactor. It will generate three plots, corresponding to the concentration of species along the catalyst bed, mole fraction of methane at the reactor exit, and the temperature profile along the reactor.
   2. The domain of simulation (‘***tspan***’) can be modified to increase or decrease the reactor domain. The variables that can be changed are, *‘****T*** *(reactor temperature)’, ‘****P*** *(initial pressure’), ‘****rho\_cat*** *(catalyst loading)’, ‘****velocity*** *(normal flow velocity)’, ‘****y0*** *(initial mole fractions)’.*
   3. The script “***equilibrium\_generator.m***” can be used to generate the best fit plots for equilibrium constant, heat of reaction, and equilibrium constant with temperature.
   4. Other scripts and functions are supplementary functions, which are called or used by the main scripts.
2. **Liquefaction**
   1. This folder has sub folders containing the scripts and functions used for getting the property values at any state. In the folder “***Get Fundamental Relations Data***”, the script “***Get\_Jacobsen\_CH4\_Data.m***” has information about the empirical fits for residual Helmholtz functions, and specific heat capacity for methane, along with other relevant information.
   2. In the root folder, the scripts “***Parts\_1\_and\_2***”, “***Part3b***”, and “***Part3a***”, are used to generate the P-v diagram, Duhring, and P-T saturation plot for methane, and the contour plot for methane. “***Part3b\_nH2***”, and “***Part3b\_CO2***” are used to generate the same plots of hydrogen and carbon dioxide respectively.
   3. The script “***Heylandt.m***” generates the state diagram for the liquefaction system (P.S. – The properties are calculated extensively for the mixture of hydrogen and methane, but represented only for methane on the T-s plot).