**The Superstructure formulation project**

The superstructure optimization code is based on GAMS modeling system (.gms), and is an update from the previous release version (2015 and 2014).

The project files are distributed as follows:

* **DOCs bin**
  + Superstructure Formulation User Manual.pdf
  + Superstructure Formulation User Manual.docs
* **Minlp bin**
  + 1\_Supr\_final\_proj.gpr
  + 2\_Super-2016-windows.gms
  + 3\_Super-2016-windows.lst
  + 4\_ADSORBER.gms
  + 5\_REGENERATOR.gms
  + 6\_Superstructure\_results.xlsx
  + **Surrogate Models bin**
    - **ADSORBERS bin**
      * **BOF bin**
        + 7\_LSO\_postopt(ADS\_BOF).gms
        + 8\_ADS\_BOF\_Variables.xlsx
        + 9\_ADS\_BOF\_Results.xlsx
      * **BUF bin**
        + LSO\_postopt(ADS\_BUF).gms
        + ADS\_BOF\_Variables.xlsx
        + ADS\_BOF\_Results.xlsx
    - **REGENERATORS bin**
      * **BOF bin**
        + LSO\_postopt(RGN\_BOF).gms
        + ADS\_BOF\_Variables.xlsx
        + ADS\_BOF\_Results.xlsx
      * **BUF bin**
        + LSO\_postopt(RGN\_BUF).gms
        + ADS\_BOF\_Variables.xlsx
        + ADS\_BOF\_Results.xlsx

First initialize gams and open the project file (file # 1, “Supr\_final\_proj.gpr”) with this you will be running all the files in the same directory. The file “super-2016-windows.gms” is the main optimization code, which includes/calls the ADSORBER.gms and REGENERATOR.gms surrogate models using “$include” function of GAMS. Files 4 and 5, correspond to the surrogate models created with the data obtained with FOQUS (ASPEN).

The bins called “surrogate models” include all the data sets for each technology. The ADS\_BOF\_Variables.xlsx includes: i) the input and output variables required for the surrogate models; ii) the maximum and minimum values used to simulate and run all the samples (the sampling scheme used was Latin Hypercube); iii) the data samplings input and output variables are included in this file.

The data sets are then used by ALAMO to obtain the surrogate models. Finally, the file LSO\_postopt(Technology).gms runs a least square optimization problem to improve the fitting of surrogate models obtained with ALAMO and the results are included in the Technology\_Results.xlsx file.