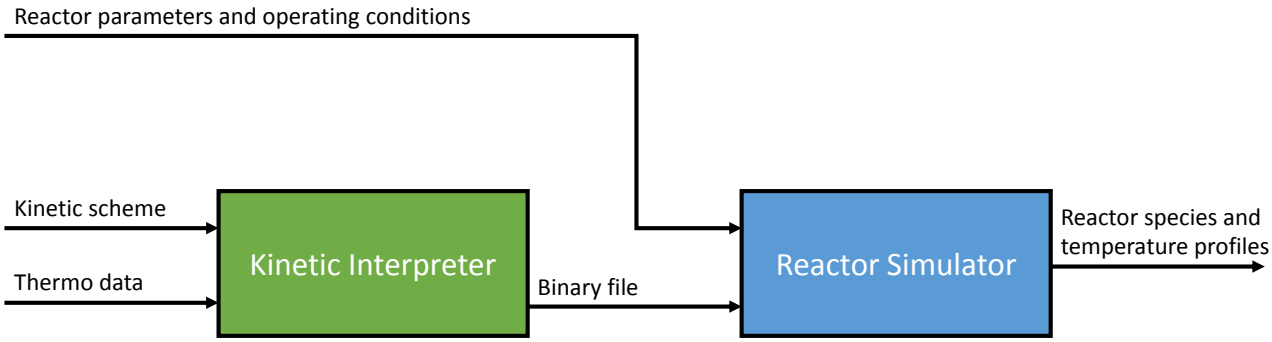
PropAro Simulator

The archive "Download_SuPER_PropAro.rar" includes the following files:

- *Lukyanov06BTX1402.kin*: kinetic file;
- *TOT1303.tdc*: thermodynamic file. The simulator has been developed to work with thermodynamic data in the form used in the NASA chemical equilibrium code. Seven polynomial coefficients for two different temperature ranges (low < 1500 K and high >1500 K temperatures) fit the specific heat, enthalpy and entropy.
- *Lukyanov06BTX1402.txt*: input file for the interpreter with the name of the kinetic and thermodynamic files;
- *Interp70.exe*: executable file of the kinetic and thermodynamic files interpreter;
- *Lukyanov06BTX1402.BIN*: binary file generated by the interpreter with the kinetic scheme;
- *PFR.dat*: input file of the reactor simulator;
- *DSMOKE70_6.exe*: executable file of the reactor simulator;
- *RUN_KS.bat*: batch file that execute the interpreter with the .kin file;
- *RUN_PFR.bat*: batch file that execute the reactor simulator with the PFR.dat input file and the binary file (kinetics + thermodynamic).



How to modify and interpret the kinetic scheme

1. Open the *Lukyanov06BTX1402.kin* file and modify stoichiometries and/or kinetic constants.
   Example: Modification of the activation energy of the 3rd reaction.

	Stoichiometry	/A/B/n/E_a/
Old:	NBUTA > BUT12 + H2	/348986/0/1/34000/
New:	NBUTA > BUT12 + H2	/348986/0/1/**31000**/

   $r_3 = k_3 * P_{NBUTA} * \theta_{free} = k'_3 * C_{NBUTA} * \theta_{free} = A_3 * 10^{B3} * T^{n3} * \exp(-E_{a,3}/RT) * C_{NBUTA} / (\sum K_{ads,i} * P_i)$

   N.B. In Appendix 1 of the reference paper (Corbetta et al., 2014), kinetic constants are reported in pressure units of measure (k), while in the kinetic file they are reported in concentrations (k' = k*R*T).

2. Launch the *RUN_KS.bat* to generate the updated binary kinetic file.

How to modify the reactor simulation

1. Open the *PFR.dat* file and modify reactor specifications and input files reported in red.

> TITLE Propane aromatization on H-ZSM-5 catalyst
>
> SPKEY C3H8
>
> STREAM 1 RATE 1.0 MOLE
>
> C3H8 1.
>
> CH4 0.
>
> SEQUE REACT 1
>
> EQUIP REACT 1
>
> TYPE=1 VOLU 163 COSV=1 TEMP=773 PRES=1 NPAS=10
>
> INPU=1 TOLR=1.E-14 RTOL=1.E-6 TOLT=1.E-8 TOLM=1.E-12
>
> RECORD H2 CH4 C2H6 C2H4 C3H8 C3H6 NBUTA BUT12 NC5 P12 NC6 ES1
>
> NC7 EPTX NC8 OLC8I BENZ TOLUO XYLO

SPKEY:	Key species that is assumed to calculate the conversion
C3H8, CH4:	Feed molar fraction composition (It is possible to specify more species)
VOLU:	Reactor volume [m^3]
	N.B. VOLU = $1/(\rho_{cat}*(1-\varepsilon)*WHSV)$, having considered a value of feed mass flowrate RATE = 1 kg/s, and defining WHSV = Feed Mass Flowrate / Catalyst Load
TEMP:	Reactor temperature [K]
PRES:	Reactor pressure [atm]
RECORD:	Species recorded in the .DTM file

2. Launch the *RUN_PFR.bat* to simulate the new reactor case study.
3. Retrieve results (temperature profiles, mass and molar fractions of the recorded species) from the .DTM file.