**GOAL**

To present and to validate a reactor model in small scale for ATR, and to describe the temperature influence on methane conversion and on yield and selectivity for the hydrogen formation, aiming to maximize the production of H$_2$.

**MATERIAL AND METHOD**

**Chemical Reaction**

- $R_1$: CH$_4$ + H$_2$O $\rightarrow$ CO + 3H$_2$  
- $R_2$: CH$_4$ + 2H$_2$O $\rightarrow$ CO$_2$ + 4H$_2$

**Equilibrium Composition**

The chemical equilibrium compositions were calculated using two distinct and classic methods: (1) Catalytic Partial Oxidation (CPOX) and (2) Steam Methane Reforming (SMR).

**Model Experimental Validation**

The model experimental validation was carried out comparing the simulated data with experimental data reported by Ayabe et al. (2003), in the same operational conditions.

**RESULTS AND DISCUSSIONS**

1. **Reaction conditions optimization**
   - The results show that, at lower temperatures, methanol total oxidation reaction is favored, generating CO$_2$. At higher temperatures, methanol reforming by CO$_2$ and steam occur, favoring the formation of synthesis gas (H$_2$ and CO).
   
2. **Mathematical modeling and parametric optimization**
   - The rate of occurrence or formation of each gas species is determined by summing up the rates of each species in all reactions.
   
3. **Equilibrium Composition**
   - The chemical equilibrium compositions were calculated using two distinct and classic methods: (1) evaluation of equilibrium constants; (2) Lagrange multipliers. Both methods result in non-linear algebraic equation, solved numerically in free software SchlabTM, through the function “solvex”.

**CONCLUSIONS**

- The proposed mathematical model has a good adjustment to the experimental data of Ayabe et al. (2003), presenting a good agreement of methane conversion and H$_2$ yields in all studied grade.
- The simulated data showed that the best reaction condition to maximize hydrogen production is around 723 K.

**REFERENCES**