Theoretical prediction of the thermodynamic effects induced by Syngas when combined with Natural gas – A Density-functional theory and canonical ensemble investigation

Abstract

Density functional theory and canonical ensemble model were used to investigate the thermodynamic properties of *Syngas* and of its mixture with natural gas as a function of temperature. The following thermodynamic potentials were obtained: internal energy, enthalpy, Gibbs free energy and entropy for temperatures between 0.5K to 1500K. We also analyzed the thermodynamic potential variations of *Syngas* and of its blends with natural gas in the *298.15* to *600K* temperature range. It was observed that carbon monoxide was the most stable *Syngas* component, possessing the ability to make *Syngas* less favorable to an increase in temperature. We also verified that *Syngas* presents properties similar to an antiknock additive for natural gas, raising its resistance to temperature increases. In addition, we also determined the Poisson coefficient, the Bulk modulus and the Shomate equation coefficients for *Syngas* and its blends with natural gas, providing a more complete thermodynamic description for these gases. Additionally, the standard thermodynamic potentials of combustion for the natural gas + *Syngas* mixtures were predicted for several *Syngas* fractions, showing that this biofuel can reduce the calorific power of natural gas. Therefore, a mixture containing around 30% *Syngas* may be useful for natural gas combustion, presenting approximately 85% of the energy released without the addition of *Syngas*.

Key-words: Syngas; Natural Gas; DFT; Thermodynamics; Temperature effect, Natural gas combustion.