Using FactSage to study the behavior of inorganic matter in thermal conversion of biomass

Françoise Defoort

CEA Grenoble DRT/LITEN/DTBH/SBRT/LTCB France

Biomass has a highly variable composition, notably in terms of inorganic species. Those species, among which alkali compounds, may greatly impact the process. Indeed, either they remain in condensed form and tend to agglomerate if liquid is present, or they volatilize as harmful species that may lead to corrosion or fouling or may affect the performance and the durability of catalysts used for syngas synthesis into Diesel Fischer−Tropsch or synthetic natural gas.

Hence, it is of crucial importance for process control to be able to predict their behavior during thermal conversion processes (combustion, pyrolysis and gasification). In particular, knowing the syngas content at gasifier exit enables forecasting of suitable gas cleaning equipment before applications. Also, depending on the technology involved, the liquid phase is highly undesirable (grate furnace, fixed or fluidized bed) or desirable (entrained flow reactor).

Thermodynamic equilibrium is now widely used in the literature to predict sufficiently high temperature processes involving chemical reactions and can be done by simulating the whole process using the minimization of the Gibbs free energy of the total system with the "Equilib" module of the Factsage software. Solutions database are necessary to take into account the occurrence of the liquid phase. Two examples of such simulations are shown. First the alkali volatilization of various biomasses during steam gasification in a fluidized bed will be shown. Second, the study of the ash behavior will be presented.

Such calculations are not very easy to carry out and there is a need to have a simple tool as scientific as possible to know if any biomass is suitable to be used in any process. Hence, we propose a tool based on simplified ternary and quaternary phase diagrams (isothermal section) calculated with the « Phase diagram » module of Factsage.

Whatever these tools are simple or sophisticated, their accuracy lies in the quality of the solution database used that is related to the presence of sufficient experimental data.