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► **To cite this version:**

G. Deffrennes, A. Pisch, I. Nuta, C. Chatillon, Françoise Defoort. Predictive tool on the equilibrium combustion ashes for adapting biomass mixtures to processes. CALPHAD XLVIII, Jun 2019, Singapour, Singapore. . hal-04877793

HAL Id: hal-04877793

<https://hal.science/hal-04877793v1>

Submitted on 9 Jan 2025

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Predictive Tool on the Equilibrium Combustion Ashes for Adapting Biomass Mixtures to Processes

G.Deffrennes¹, A.Pisch¹, I.Nuta^{1*}, C.Chatillon¹, F.Defoort²

¹ Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

² CEA LITEN/DTBH/STBH/LPB, 17 Av de Martyres, Grenoble, France

e-mail address of corresponding author: ioana.nuta@grenoble-inp.fr

Key words: K-O, CaO-K₂O, biomass, ash

This work is to implement a tool for predicting the behavior of any new used biomass (agricultural waste) or mixture of biomass, during combustion / gasification in a thermochemical process for the production of energy or biofuel. This tool will be based on a thermodynamic equilibrium simulation with a reliable and quality thermodynamic database. In the specific case of biomass burning, this base you can hold up to 20 chemical elements, but the predominant system is the ternary system K₂O-CaO-SiO₂ (> 90% mass of biomass ash). The balance of the ternary system as well as the phases and related compounds are very well known, especially in the field of alkali-rich composition K₂O for which no experimental data exist. Indeed, it is very difficult to develop and characterize samples in this area because of the high reactivity of alkali oxides with respect to moisture and CO₂ (g) in the ambient air. In addition, K₂O(s) does not exist commercially and must be synthesized beforehand. The classical approaches encountered in the literature for such a prediction use empirical tools based on the chemical composition of biomass (K: Si ratio for example) by analogy with the criteria of coal [1,2]. These criteria may give some trends, but they fail as soon as the raw material is outside the composition range of the model.

The thermochemical conversion of biomass is a thermal process where it can be reasonable to consider that the thermodynamic equilibrium can be reached because of the high temperatures (800-1000 °C, 1300-1500 °C) and the long dwell times put involved in the processes. This project proposes to predict the behavior of biomass ash using thermodynamic equilibrium calculations. A database of stoichiometric compounds (8-20 elements) is already used in the literature to study the volatilization of inorganic species for coal [3] or biomass [4]. On the other hand, a database comprising the liquid and solid solutions is necessary for the predictions of agglomeration and condensation because they involve liquid phases. Such bases have already been

used in the literature for coal but not for biomass [3,4]. Indeed, the major elements of the coal ash (Al, Ca, Fe, Si, Mg) are not the same as for the biomasses (Ca, K, Si, P, Mg) in particular the presence of alkalis (K, Na) significantly increases the amount of liquid phase. This work would propose:

- Synthesis of pure K₂O + data revision thermodynamic of the K-O system
- Experimental thermodynamic study e and theoretical of the binary phase diagram CaO-K₂O
- Experimental thermodynamic study e and theoretical of the phase diagram of the CaO-K₂O-SiO₂ ternary system
- Insertion of thermodynamic data of ternary CaO-K₂O-SiO₂ in the complete database + application calculations.

In our contribution, we will present first results on the K-O system and selected results in the binary and ternary systems.

References

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Biographical Note

I.Nuta, chemical engineer, is research scientist on thermodynamics of the gaseous phase using Knudsen effusion method coupled with mass spectrometry and calorimetry. Her research activity is about the study of the thermochemical properties of compounds mainly for energy production and storage.