Phytoremediation and Emission Control

Introduction

- Climate change urges us to face global energy issues and investments are made to reduce greenhouse gases and to develop renewables.
- **Biomass** is one potential solution and **phytoremediation** can be used to clean heavy metal-contaminated lands and supply growing energy demand.
- Ca-based sorbent (**limestone** | $CaCO_3$) is used during **combustion** to **ab/adsorb** and recover metals, working better in **fluidised-bed reactors**.
- Thermodynamic model based on **Gibbs free energy** minimisation to predict the products (MATLAB) and Validation using ASPEN PLUS.

Objective

- **Thermodynamic** modelling of using **Ca-based sorbents** for **heavy metal** emission control during contaminated biomass combustion.

Methodology

- Several MATLAB and ASPEN models were developed, from combustion of CH_4 to complex biomass plants.
- Two case studies were analysed by applying the model created.

1. Heavy Metals and Phytoextraction

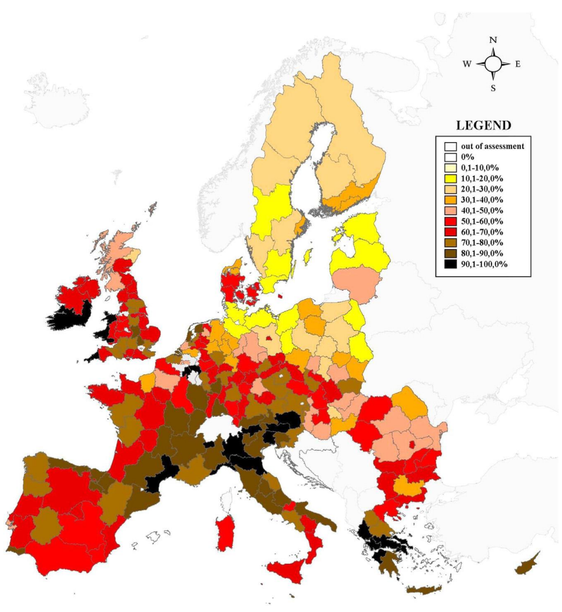

Fig. 1. Percentage of samples with **As** concentration above the threshold value

Metal	Health issues	Permissible limit (mg/kg)
Arsenic (As)	Skin poisoning, kidney, Central Nervous System	20
Lead (Pb)	Mental lapse	50
Mercury (Hg)	CNS, liver, heart, kidney damage	2
Cadmium (Cd)	Kidney, liver, heart	3
Nickel (Ni)	Carcinogenic in excess	50

Table 1. Heavy Metals in contaminated soils and Risks

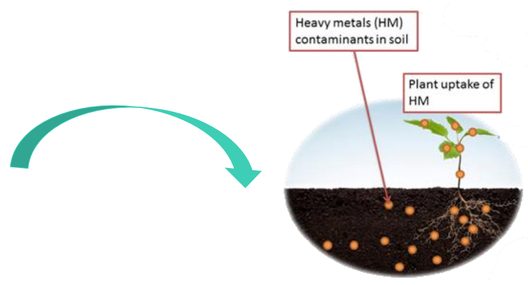

Fig. 2. Phytoextraction of Heavy Metals

2. Combustion

The model created enables the user to obtain which are the **most possible compounds** that are produced in the combustion of a certain type of biomass and what is the ab/adsorption rate of the heavy metals presented.

Gibbs free energy minimisation equation

$$G = \sum_{\alpha} \sum_{k} n_k^{\alpha} \mu_k^{\alpha}$$

- G : Gibbs free energy (J)
- n_k^{α} : moles of k component in α phase
- μ : chemical potential (J/mol)

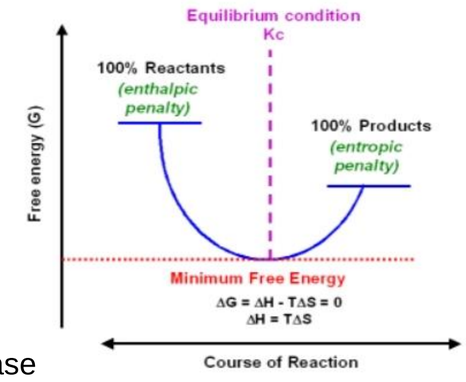

Fig. 4. Gibbs Free Energy Minimisation

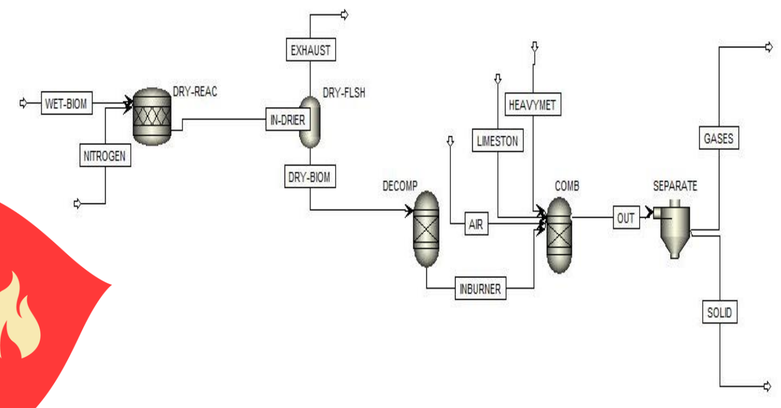

Fig. 5. Aspen Model used for validation of the Matlab code

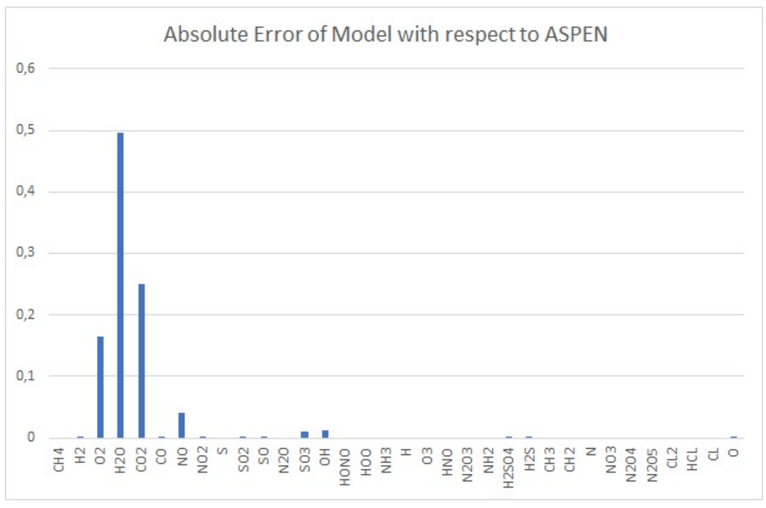

Fig. 6. Absolute error between Matlab results and Aspen

3. Case Studies

In phytoextraction two main types of plants are commonly used, which are:

- **Hyperaccumulators**: plant species with high level of accumulation
- **Short Rotation Coppices (SRC)**: densely planted, high yielding plants .

The performance of one hyperaccumulator -*Pteris Vittata*- and one SRC -Willow *Salix*- was analysed, obtaining their economic feasibility.

Species	Harvested Metals	Phytomining and Energy output Profit (£/ha)
P. Vittata	Pb, Cu	1187
Willow *Salix*	Pb, Cr, Cu, Cd	2201
Sun flower	Cu, Cd	2319
Miscanthus	Pb, Cd	1681

Table 2. Some examples of plants and economic assessment

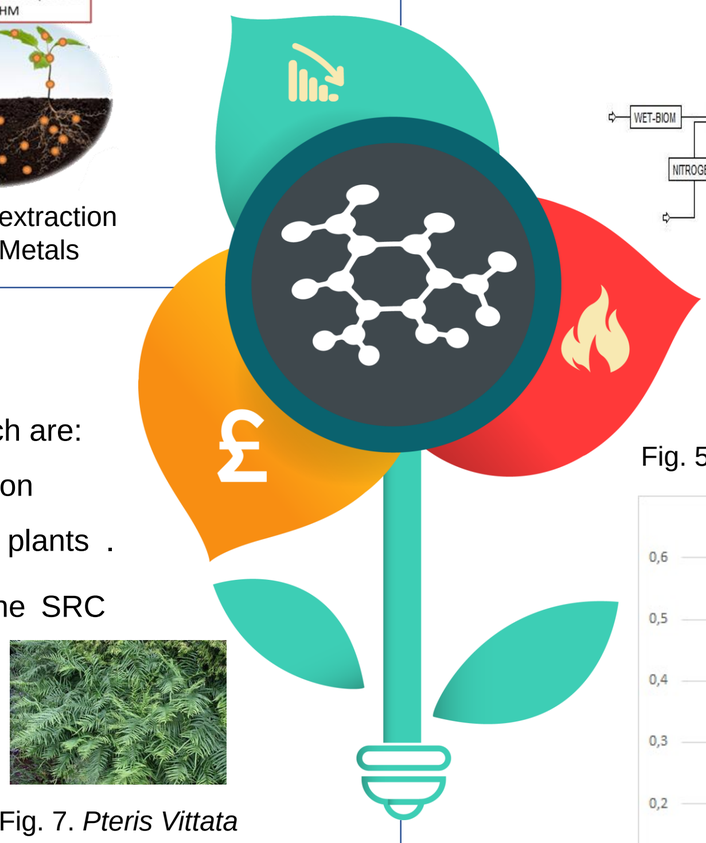

Fig. 7. *Pteris Vittata*

Fig. 8. Willow *Salix*

Conclusion

Researches on the main issues concerning the contaminated lands and the plant species used were made. Data concerning biomass, heavy metals, sorbents and thermodynamic parameters were largely gathered through the whole process. A thermodynamic model has been developed and coded into Matlab. The results were confirmed with Aspen, providing an efficient method to predict key outputs and to evaluate profitability.

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