Prediction of heating value of biomass fuel and ash melting behaviour using elemental compositions of fuel and ash

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Introduction

Biomass has increasing importance as fuel.

Biomass is renewable, and incineration does not affect the overall CO_2 balance in the atmosphere.

THIS WORK

PCA has been applied for a cluster analysis of biomass samples, based on elemental compositions*.

Two technological properties

- **heating value of biomass[1],**
- **softening temperature of ash[2] from biomass incineration**

have been modeled by the elemental compositions of the samples*, using OLS, PLS and a KNN-approach.

[1] ***HHV*, higher heating value** (gross calorific value) is the enthalpy of combustion including the condensation enthalpy of water; *HHV* has been measured by bomb calorimetry.

[2] ***SOT*, softening temperature** (deformation temperature) is the temperature at which the first signs of rounding, due to melting, of the tip or edges occur; *SOT* has been measured by a heating microscope.

* K. Reisinger, C. Haslinger, M. Herger, H. Hofbauer: BIOBIB a database for biofuels, THERMIE Conference: Renewable Energy Database, Harwell UK, 1996.

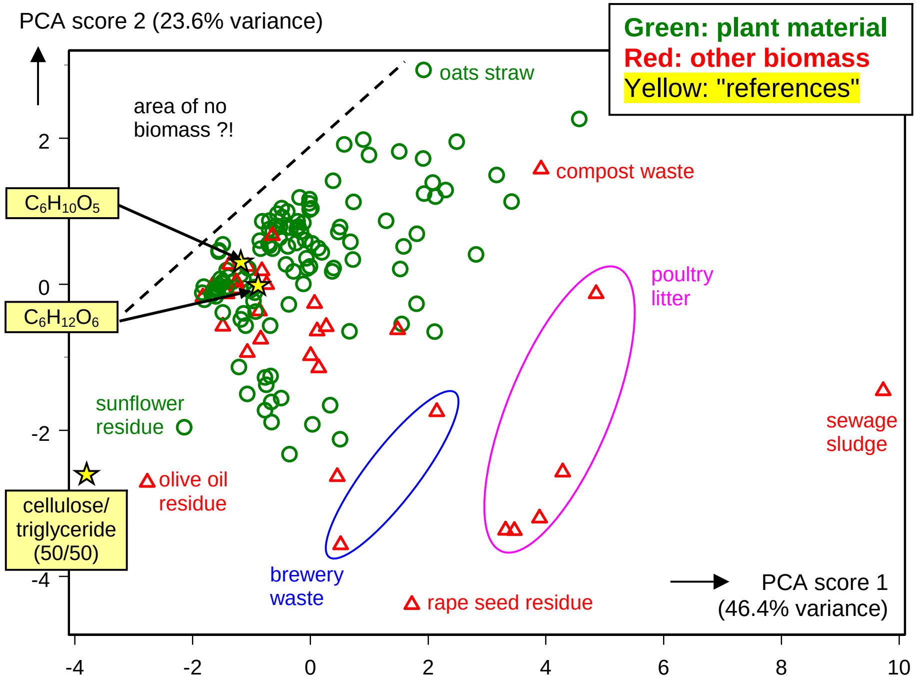
Cluster analysis of biomass

n = 154 biomass samples of very different origin

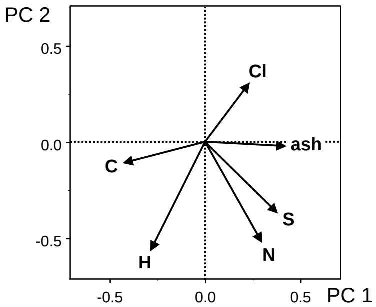
Different types of wood material, bark, grass, rye, wheat, rape, sunflower, reed, brewery waste, poultry litter, sewage sludge.

p = 6 features

Mass % of C, H, N, S, Cl, ash in dry biomass (autoscaled).



PCA loading plot



Correlation coefficients

	C	H	N	S	Cl	ash
C	1.00	0.49	-0.31	-0.44	-0.24	-0.69
H	0.49	1.00	0.16	-0.11	-0.39	-0.43
N	-0.31	0.16	1.00	0.57	0.10	0.41
S	-0.44	-0.11	0.57	1.00	0.12	0.57
Cl	-0.24	-0.39	0.10	0.12	1.00	0.31
ash	-0.69	-0.43	0.41	0.57	0.31	1.00

Heating value of biomass

n = 122 biomass samples from plant materials

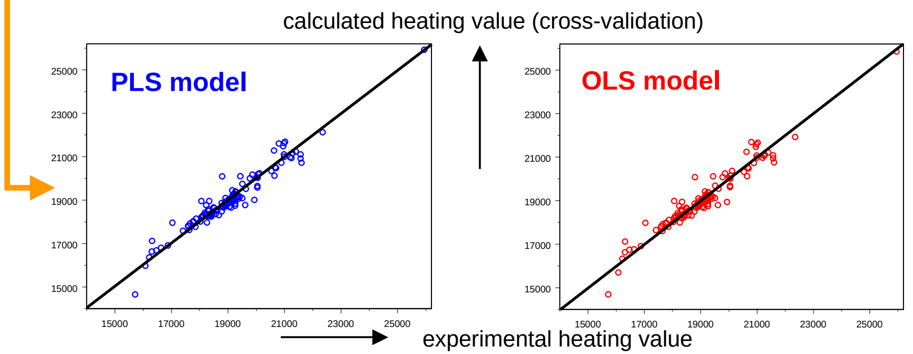
Wood, wood waste, bark, miscanthus grass, rye, wheat, rape, sorghum, sunflower, alfalfa, maize, flax, ...

p = 1 - 25 features

7 basic features are mass% of C, H, N, S, O, Cl, ash in dry biomass; derived features are square and cross terms, ratios, and logarithms.

p	*m*	Features	Meth.	R^2_{cv}	*SEP*	Remarks
1	1	C	OLS	0.887	476	
4	3	C, C^2, H, N	OLS	0.930	376	
5	3	C, C^2, H, C*H, N	OLS	0.935	362	BEST MODELS
5	3	C, C^2, H, C*H, N	PLS	0.935	361	4 components
6	6	C, H, N, S, Cl, ash	PLS	0.908	429	5 components
25	6	C, H, N, S, Cl, ash, derived features	PLS	0.928	379	14 components
5	5	C, H, N, S, O		0.814	777*	Boie (1957)
4	4	C, H, S, O		0.807	837*	Dulong (1912)
6	6	C, H, N, S, O, ash		0.807	851*	Mason (1983)
4	4	C, H, S, O		0.736	910*	Mott (1940)
5	5	C,H, N, S, O		0.762	990*	Wilson (1972)

m, number of analytical measurements used; R^2_{cv}, *SEP (standard error of prediction)* from leave-one-out cross validation; * bias-corrected models, see Summary



Softening temperature of ash

n = 99 ash samples from biomass incineration

p = 8 features

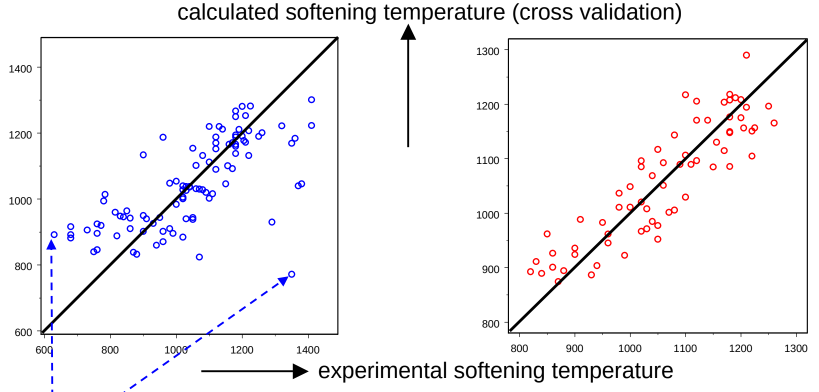
8 basic features are relative mass concentrations of Na_2O, K_2O, MgO, CaO, Al_2O_3, SiO_2, P_2O_5, Fe_2O_3 (sum = 100); derived features are concentration ratios, square and root terms.

p	m	Features	Meth.	R^2_{cv}	*SEP*	Remarks
1	4	$(Na_2O + K_2O) / (MgO + CaO)$	OLS	0.320	153	
8	8	basic features	PLS	0.412	142	4 components
20	8	basic + derived features	PLS	0.422	142	3 components
8	8	basic features	KNN*	0.467	135	5 neighbors, better than PLS
4	4	K_2O, CaO, Al_2O_3, P_2O_5 (sum = 100)	PLS	0.780	57	**BEST MODEL** (n=67, obvious outliers removed)

* mean of *SOT* from 5 nearest neighbors (Euclidean distance); 5 neighbors yield best prediction.
m, number of analytical measurements used; R^2_{cv}, *SEP (standard error of prediction)* from leave-one-out cross validation.

KNN approach (5 neighbors)
n = 99, p = 8

PLS model from subset
n = 67, p = 4



Typical outliers - probably due to experimental errors - show very different *SOT* values for 5 nearest neighbors.

Summary

Higher heating value of dry biomass consisting of plant material

HHV [kJ/kg] =

= 1.87 C^2 - 144 C - 2820 H + 63.8 $C*H$ + 129 N + 20147 (OLS)

= 5.22 C^2 - 319 C - 1647 H + 38.6 $C*H$ + 133 N + 21028 (PLS)

C, H, N are mass% carbon, hydrogen, nitrogen, resp., in dry biomass.

The two models have quite different regression coefficients, but almost identical performances (*SEP* = 362 and 361, R^2_{cv} = 0.935).

These models explain deviations from the average; they are applicable to samples similar to the used biomass samples.

SEP = 361 kJ/kg corresponds to 1.4 - 2.3% of *HHV*.

In contrary, most models from literature (Boie, Dulong,...) use an intercept of zero. Bias-corrected predictions of these models still show much higher *SEP* with 777- 990 kJ/kg than the new models.

Softening temperature of ash from biomass

SOT [^oC] =

= 1.81 $c(CaO)$ + 4.20 $c(Al_2O_3)$ - 2.41 $c(K_2O)$ + 5.31 $c(P_2O_5)$ + 1017

c(.) are relative mass concentrations in ash, normalized to sum 100.

This model is useful for plausibility checks of experimental results, and allows semi-quantitative estimations of softening temperatures.

SEP = 57 ^oC corresponds to 4 - 9% of *SOT*.