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The importance of the relationship between lignin and carbohydrate contents when predicting biomethane potentials from lignocellulosic biomass

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Introduction

Why?!  
- We are aiming to find the best way of finding predicted BioMethane Potential (pBMP) from compositional data of a lignocellulosic biomass – without making time-consuming BMP tests.
- We are questioning the use of standard linear regression, or multiple linear regression, of the type $pBMP = \alpha_0 + \sum \beta_i x_i$ such as proposed previously [1, 2], these models often only find lignin to be significant to pBMP.
- The previous models described the data adequately, but were not intuitive and did not go well with the theoretic background of anaerobic digestion (e.g. could not show significance of carbohydrates).

What's new?!  
- We introduce a new way of statistically describing the relationship of biomass constituents and pBMP – The Mixture Model – this was previously used when describing effects of chemical mixtures. In that way we can show the true importance of each of the biomass constituents.
- In mixture models, the variables are proportionate nonnegative amounts of different constituents $0 \leq x_i \leq 1, i = 1, 2, ..., q$. In this case the variables are biomass constituents: Cellulose $(X_1)$, hemicellulose $(X_2)$, carbohydrates $(X_3 + X_4)$, lignin $(X_5)$.
- In mixture models the variables sum up to one, $\sum x_i = 1$. Therefore what is known as residuals when looking at biomass composition is included in the model – in this case everything which is not carbohydrates or lignin is characterized as residuals, $x_0 = 1 - (X_3 + X_4 + X_5)$.
- We test the linear model for mixture designs $Y = \sum \beta_i x_i$ as well as the quadratic model for mixture designs $Y = \sum \beta_i x_i + \sum \gamma_i x_i x_j$ as developed by Henry Scheffe and peers from 1953 and onwards [4,5].

Results

How was the data collected?!  
- We assessed data from peer reviewed literature, with the prerequisites that the data should include BMP as well content of cellulose, hemicellulose and lignin, and that the biomass in question should be lignocellulosic.
- We collected 49 data sets from literature from a broad spectrum of different lignocellulosic biomasses.
- Furthermore, we prepared 16 data sets for this study, summing to a total of 65 data sets.
- Data and references are not shown – but will be displayed in following paper submission.

Comparison of models:

- Models are compared on the basis of: significance of regression coefficients, $R^2$-values, P-values, and relative Root Mean Square Error $rRMSE = (\sum (\tilde{y} - y)^2/n)/\text{mean}(BMP)$, see table below.
- Notice that the $rRMSE$ – which shows how far the pBMP’s are from the measured BMP’s – is fairly similar for the different models.
- Also notice, that the $R^2$ - a measure of how well observed outcomes are predicted by the model – is much higher in the mixture designs presented in this study.

Discussion

Why are the previous models both wrong and correct?!  
- The inherent mathematical connection between the mixture models and the models with intercept is described by the following calculations:

$$pBMP = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + \beta_5 X_5$$

- The problem by the latter equation is that both $\beta_1$ and $\beta_2$ are positive and in the same order of magnitude then $\beta_1 - \beta_2 - \beta_3$ will be small, thus it will seem insignificant. It might even be negative even though that is unintuitive and contrary to AD theory.
- Likewise, $\beta_4 - \beta_3 - \beta_5$ will be a large negative variable with high significance since $\beta_3$ already is a negative regressor – Thus, the role of lignin have been exaggerated!
- These problems are linked to a concept known as multicollinearity – an effect which is known to interfere with the significance of variables.

What is the consequence of not summing to 1?!  
- The relative nature of all compositional data which have units of w/w% or g/100 g TS, are not taken into account.
- The effects of methane yielding carbohydrates cannot be proved significant.
- Residuals, including methane yielding biomass constituent like lipids and proteins, are not taken into account.
- Instead the effects of carbohydrates and residuals are hidden in the intercept ($\alpha$)
- Since the variables (biomass constituents) have the same order of magnitude, and since they have an underlying connection, multicollinearity is a problem.

Why is our model more intuitive?!  
- Since the biomass constituents that in theory should be energy yielding are positive (e.g. cellulose), while lignin which is known to have an inhibitory shielding effect on BMP is negative.
- Since the pBMP is not only determined by lignin content.
- Regression coefficients for contents of cellulose, hemicellulose, lignin, and residuals are all highly significant.

Can we prove that the interactions between lignin and carbohydrates are important?!  
- When testing the quadratic model for mixture designs $pBMP = \sum \beta_i x_i + \sum \gamma_i x_i x_j$ none of the blending terms were significant.
- Thus a linear mixture model is preferred, and we cannot prove that the interactions are important.
- However, a quadratic model for mixture designs might be more relevant on a more homogenous data set, E.g. with only one lignocellulosic biomass type.

Selected references


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