GHENT UNIVERSITY

Model based assessment of anaerobic digestion of lignocellulose containing waste materials

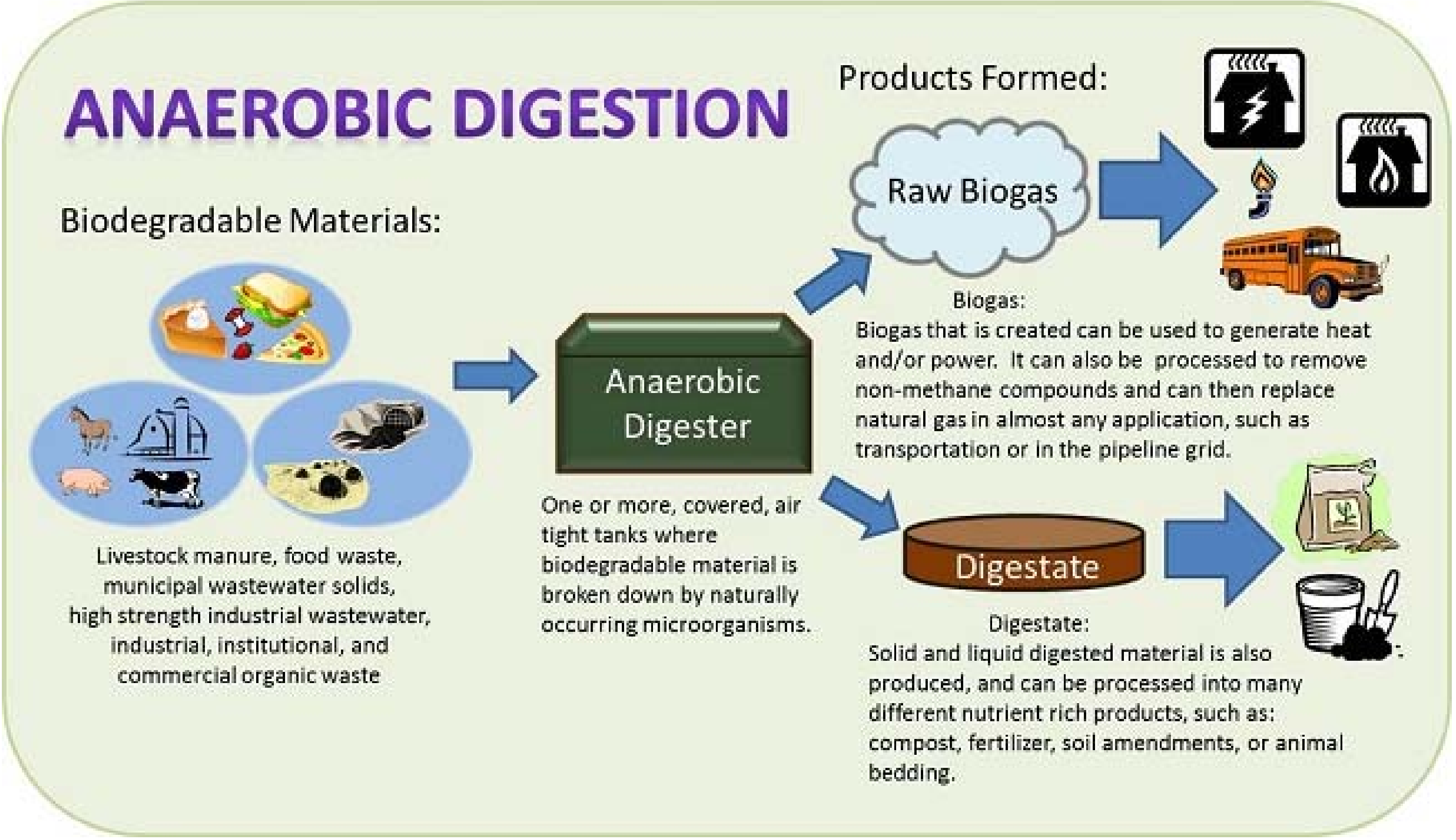
S.W.H. Van Hulle[1], M. Schroyen[1,2] & K. Raes[2]

[1]Department of Green Chemistry and Technology, Ghent University, Campus Kortrijk, Belgium
[2]Department of Food technology, Safety and Health, Ghent University, Campus Kortrijk, Belgium

Outline

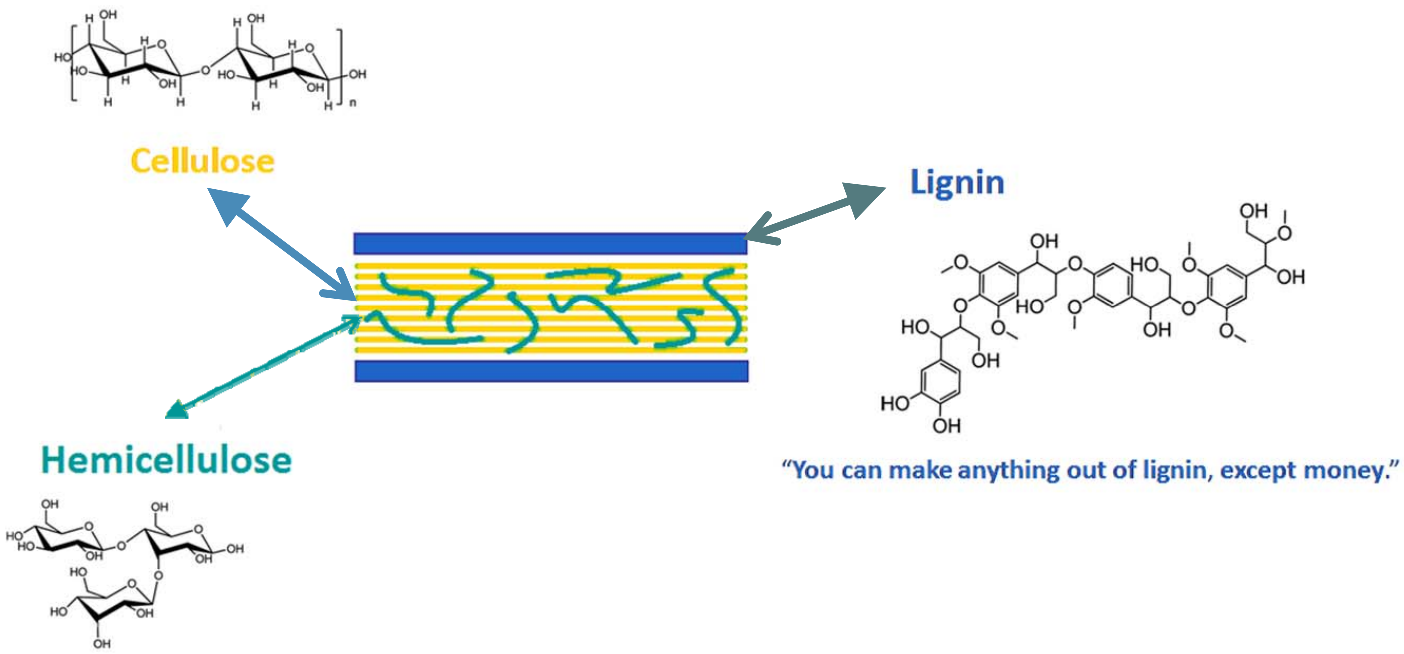
- Introduction
- Model development
- Model application

Anaerobic digestion (AD) of (solid) waste



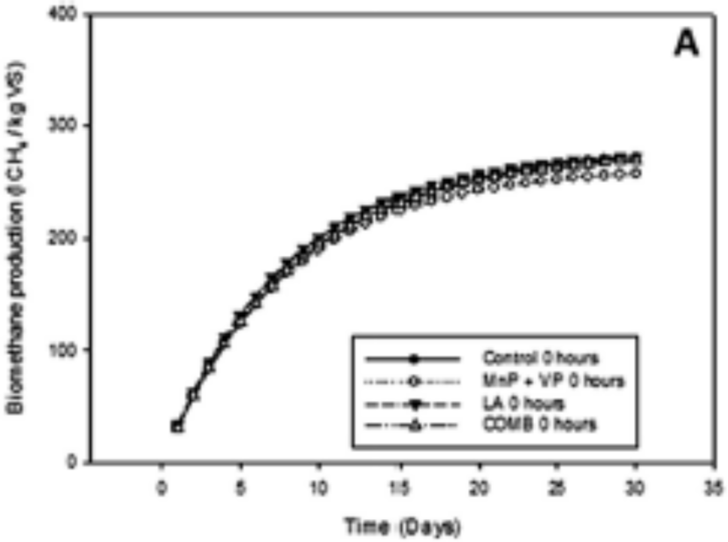
GHENT UNIVERSITY

Lignocellulosic substrates (LS)



Lignocellulosic substrates (LS)

- E.g. agricultural residues
- Reduction in biogas production



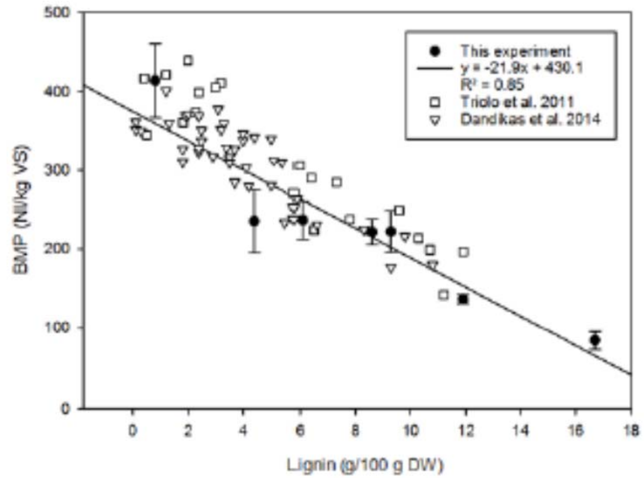
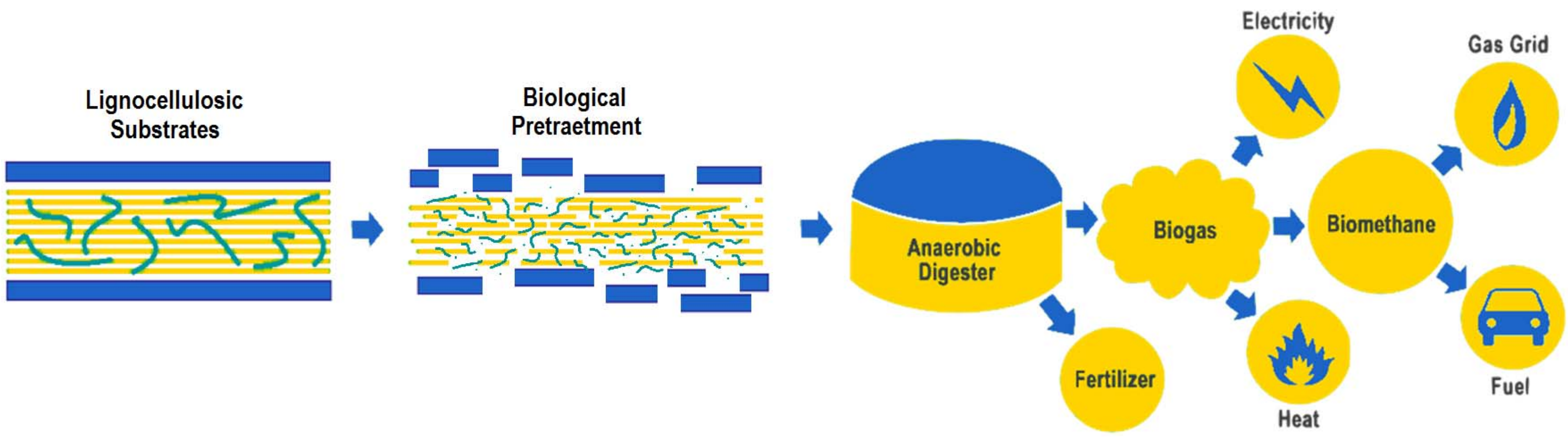


Figure 2.5: Biomethane potential values of recent studies compared to experimental results from this study in relation with the lignin values of the selected substrates. (Dandikas et al. 2014; Triolo et al. 2011).

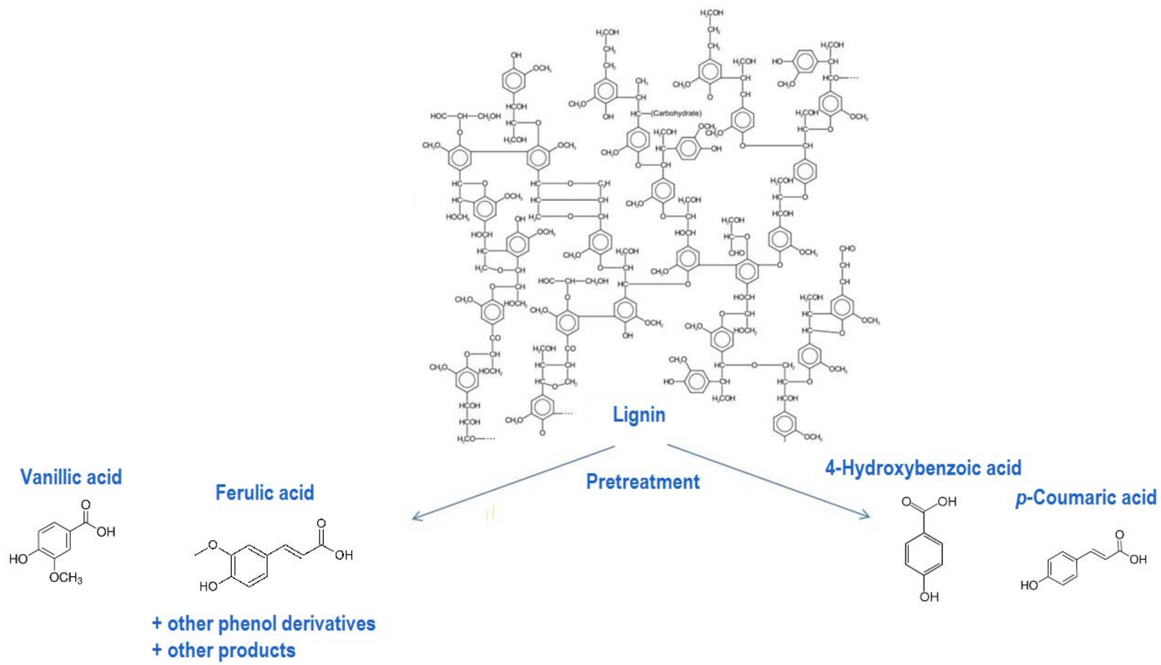
(Biological) pretreatment

- Improve anaerobic digestion



(Biological) pretreatment

- Pretreatment causes formation of inhibiting phenolic compounds



(Biological) pretreatment

- Effect on hydrolysis rate (k_1) of miscanthus (high lignin content)

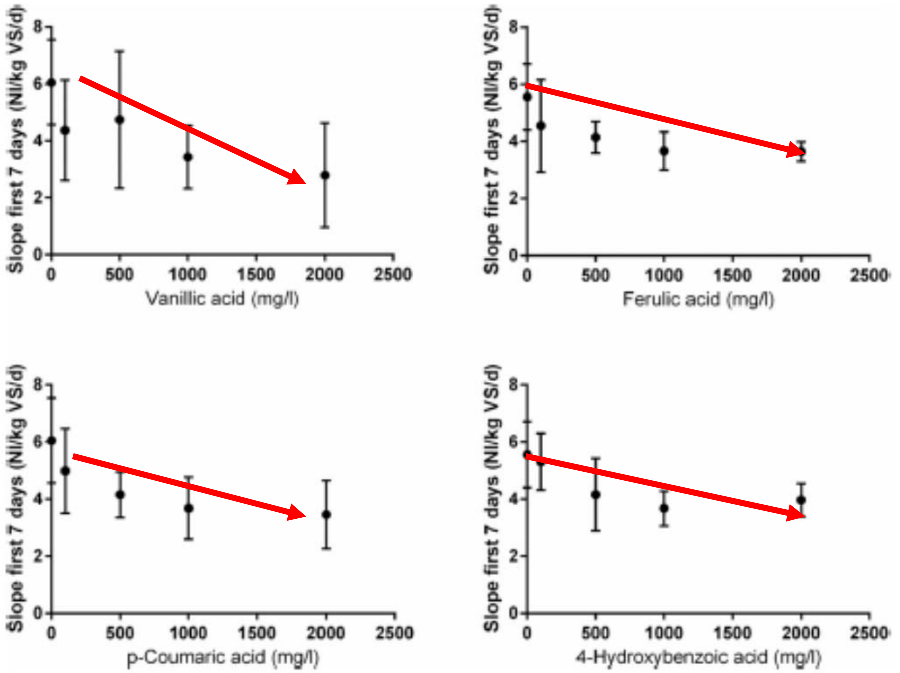


Fig. 4. The initial slope of biogas production of miscanthus as substrate with various added concentrations of the different phenolic components. ($n = 3$).

(Biological) pretreatment

- Effect on hydrolysis rate (k_1) of hemp straw (low lignin content)

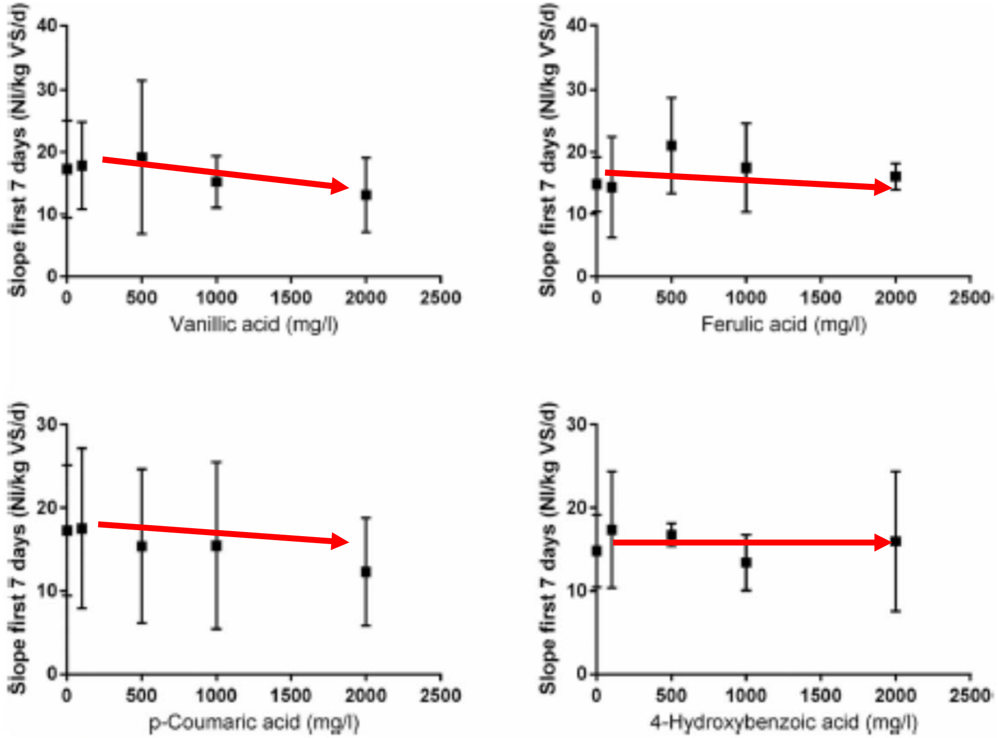


Fig. 5. The initial slope of biogas production of hemp straw as substrate with various added concentrations of the different phenolic components. ($n = 3$).

Modelling of AD for LS

- Simplified AD model
  - Developed previously for AD of manure
  - VSS -> VDS -> VFA -> CH_4
  - COD based
  - Upgraded with effect of pretreatment
    - Lignin content (C_L) -> reduction of maximal biogas production and hydrolysis rate
    - Phenolic components (C_P) -> reduction of hydrolysis rate

Simplified AD model

- VSS -> VDS -> VFA -> CH_4
- Gujer Matrix:

Table 1
Gujer Matrix of the anaerobic digestion model, with inhibition of lignin and phenolic compounds, used in this work.

Process	VSS	VDS	VFA	CH_4	X_1	X_2	Process rate
Hydrolysis	−1	1					$k_1\,[VSS]\,\frac{K_L}{K_L+C_L}\,\frac{SP*C_P+K_I}{C_P+K_I}$
VFA formation		−1	1-Y_1		Y_1		$k_2\,\frac{[VDS]}{k_3+[VDS]}\,[X_1]$
CH_4 formation			−1	1-Y_2		Y_2	$k_4\,\frac{[VFA]}{k_5+[VFA]}\,[X_2]$
Decay acidogenic bacteria					−1		$b_1\,[X_1]$
Decay methanogenic Archaea						−1	$b_2\,[X_2]$

Hydrolysis rate : function of C_L and C_P

Simplified AD model

- VSS -> VDS -> VFA -> CH_4
- Parameters values used:

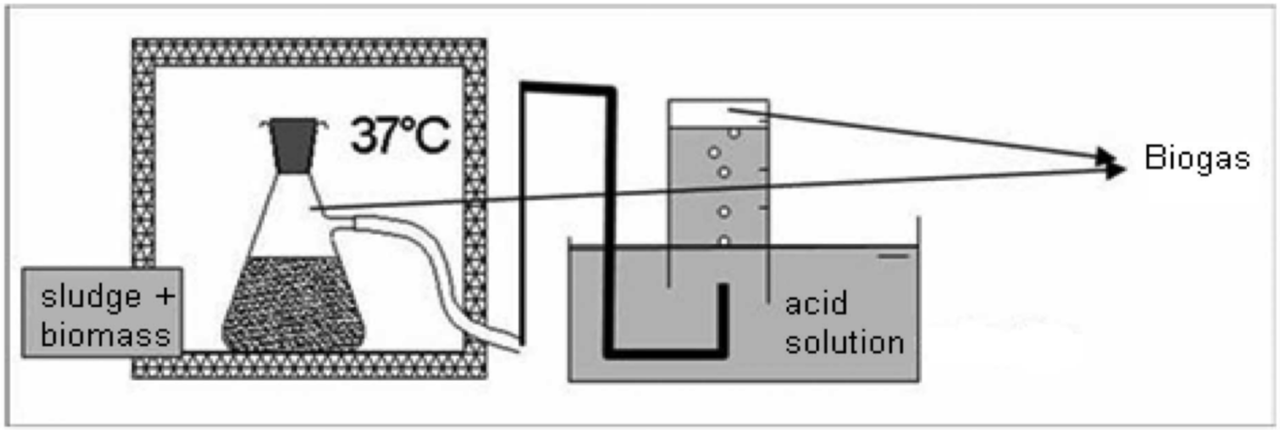
Table 3
Parameter values for the kinetic model used in this study.

Parameter	Value
k_1	$0.2\ d^{-1}$
k_2	$8\ d^{-1}$
k_3	10 gCOD/l
k_4	$8\ d^{-1}$
k_5	1.2 gCOD/l
b_1	$0.16\ d^{-1}$
b_2	$0.16\ d^{-1}$
K_I	150–3000 mg/g
K_L	35 g/100 g

Hydrolysis rate constant: much lower than e.g. studies with waste water (cfr. ADM1)

Simplified AD model

- VSS -> VDS -> VFA -> CH_4
- Model tested with AD batch tests with different substrates
  - V: 250 ml
  - Substrate to inoculum ratio of 0.5 (g VS/g VS)



Simplified AD model

- Effect of C_L
  - BMP ↓ if C_L ↑

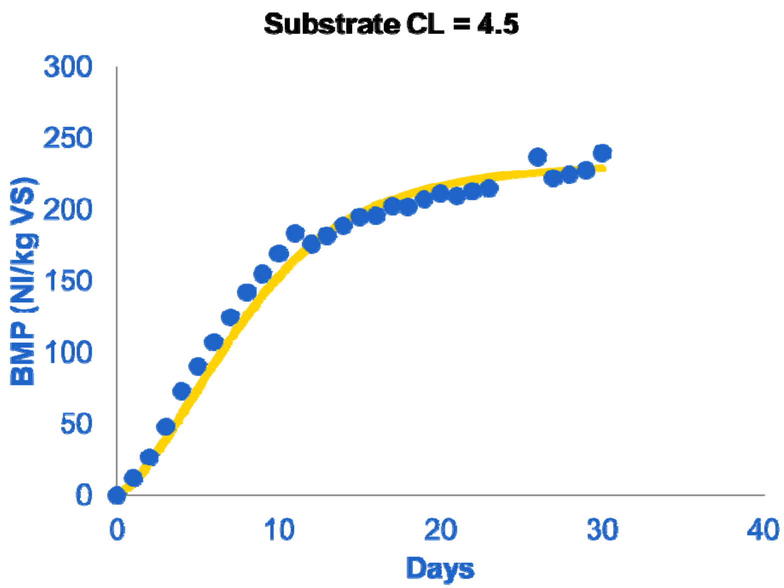
Substrate	BMP (Nl* /kgVS)	VSS (gCOD/l)	C_L (g/100 g)
Ensilaged maize	413.9	40.0	0.8
Corn stover	242.4	22.8	4.5
Wheat straw	247.1	22.8	6.0
Flax straw	233.1	21.6	8.6
Hemp straw	237.8	21.6	9.2
Miscanthus	144.5	13.2	12.0
Willow	88.6	8.0	17.0

* Nl stands for normal liter.

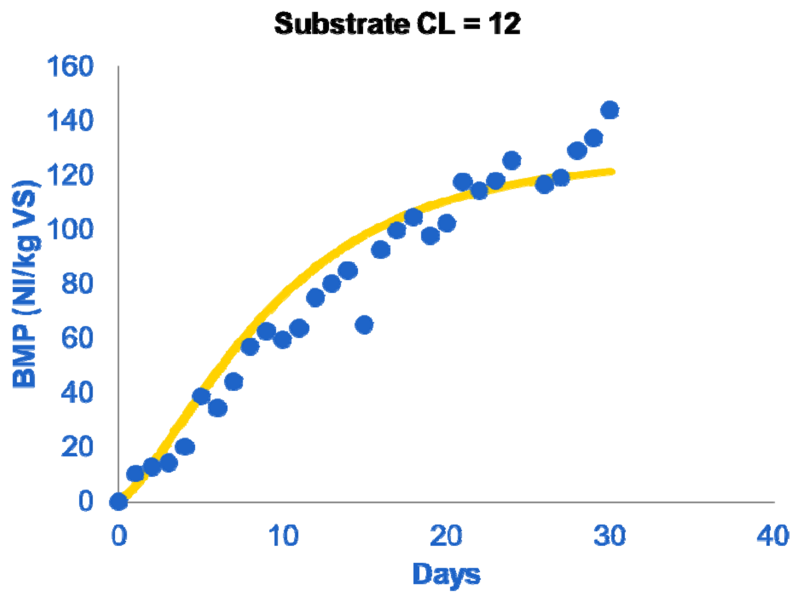
Simplified AD model

- Effect of C_L
  - Hydrolysis rate ↓ if C_L ↑

$$k_1\,[VSS]\,\boxed{\frac{K_L}{K_L + C_L}}\,\frac{SP + C_P + K_I}{C_P + K_I}$$



Corn stover



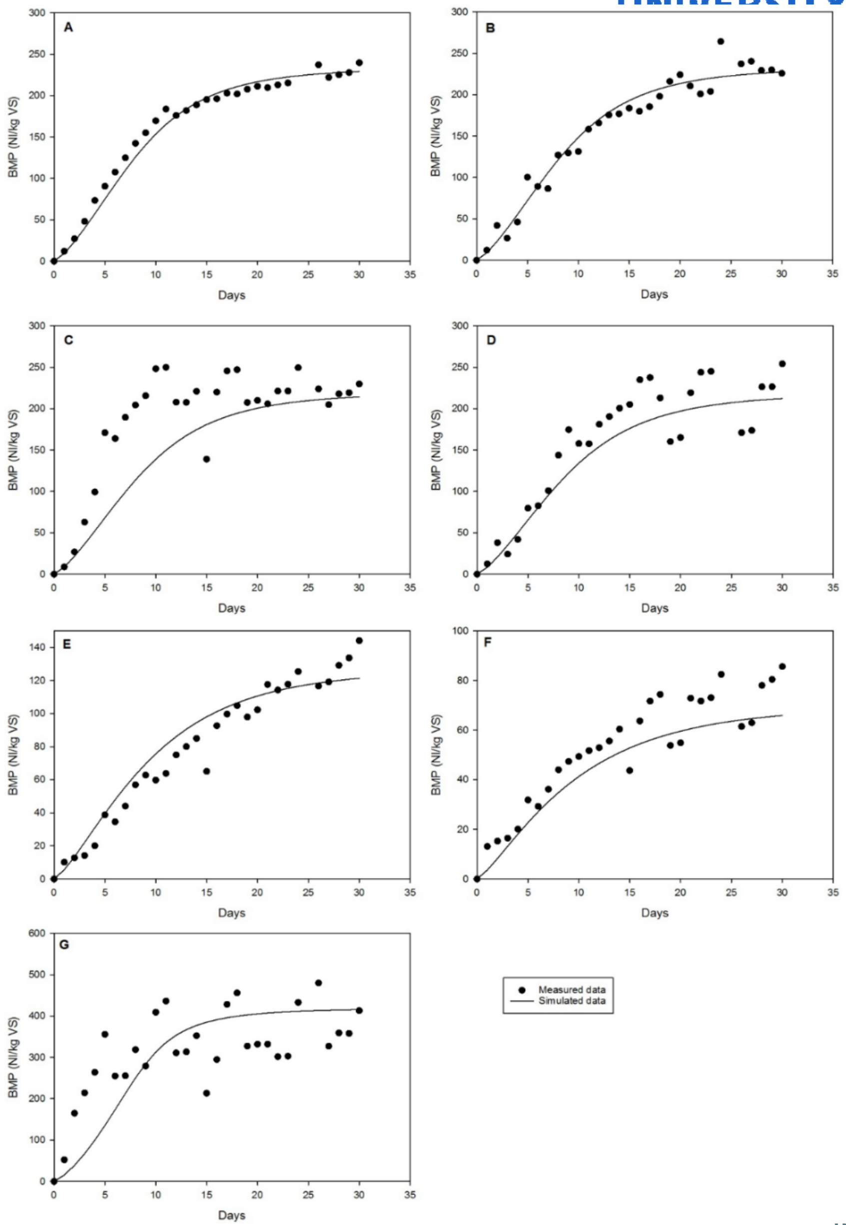
Miscanthus

Model application

- Effect of C_L
  - C_L: 0,8 -> 17 g/100g
  - TIC: 0,03-0,14 < 0,3: OK

$$TIC = \frac{\sqrt{\sum_i (y_i^2 - y_{i,m}^2)}}{\sqrt{\sum_i y_i^2} + \sqrt{\sum_i y_{i,m}^2}}$$

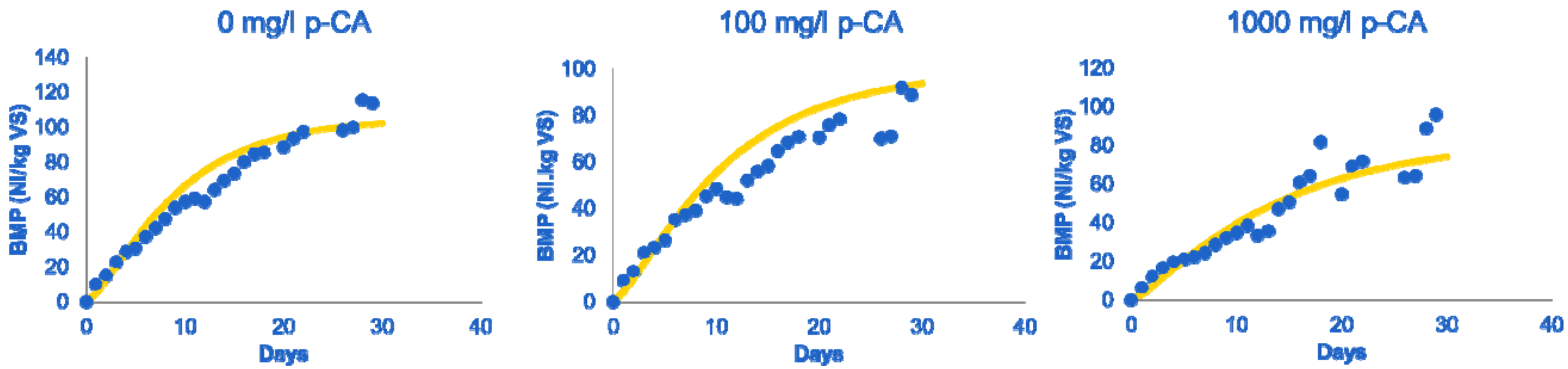
- Low C_P



Simplified AD model

- Effect of C_P
  - Hydrolysis rate ↓ if C_P ↑

$$k_1\,[VSS]\,\frac{K_L}{K_L+C_L}\,\boxed{\frac{SP*C_P+K_I}{C_P+K_I}}$$



Miscanthus

Model application

- Effect of C_P
  - 4 phenolic compounds at 4 concentrations:
    - SP=0,4:
      - VA: vanillic acid
      - PCA: p-coumaric acid
    - SP=0,8
      - FA: ferulic acid
      - HBA: 4-hydroxybenzoic acid)

Table 6.4: Measured and simulated hydrolysis rate (k_h), and measured and simulated BMP of the anaerobic digestion of hemp straw with the addition of the different phenolic compounds at concentrations of 100, 500, 1000 and 2000 mg/l (VA = vanillic acid, FA = ferulic acid, PCA = *p*-coumaric acid and HBA = 4-hydroxybenzoic acid) (n=20)

Phenolic compound	Initially added concentration (mg/l)	Measured BMP (Nl/kg VS)	Simulated BMP (Nl/kg VS)	Measured hydrolysis rate (Nl/kg VS/d)	Simulated hydrolysis rate (Nl/kg VS/d)
VA	0	114	102	5.8	7.3
	100	81	93	3.2	6.0
	500	87	79	3.3	4.6
	1000	81	73	3.2	4.2
	2000	74	70	1.0	4.0
FA	0	87	73	5.6	5.5
	100	107	72	6.5	5.3
	500	86	70	5.6	5.1
	1000	81	69	4.7	5.0
	2000	92	68	4.3	4.8
PCA	0	114	102	5.8	7.3
	100	89	93	5.2	6.0
	500	92	79	3.8	4.6
	1000	96	73	3.3	4.2
	2000	81	70	3.5	4.0
HBA	0	87	73	5.6	5.5
	100	90	72	6.5	5.3
	500	82	70	2.2	5.1
	1000	84	69	5.0	5.0
	2000	96	68	4.9	4.8

Model application

- Effect of CP
  - 4 phenolic compounds at 4 concentrations:
    - TIC < 0,3

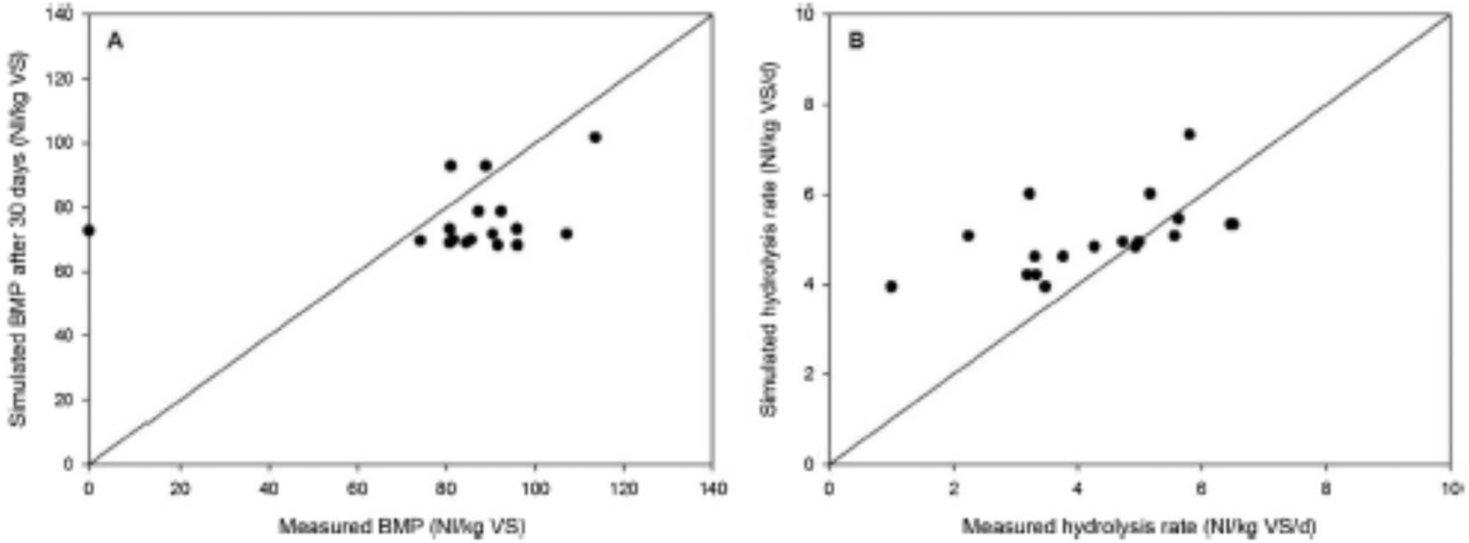
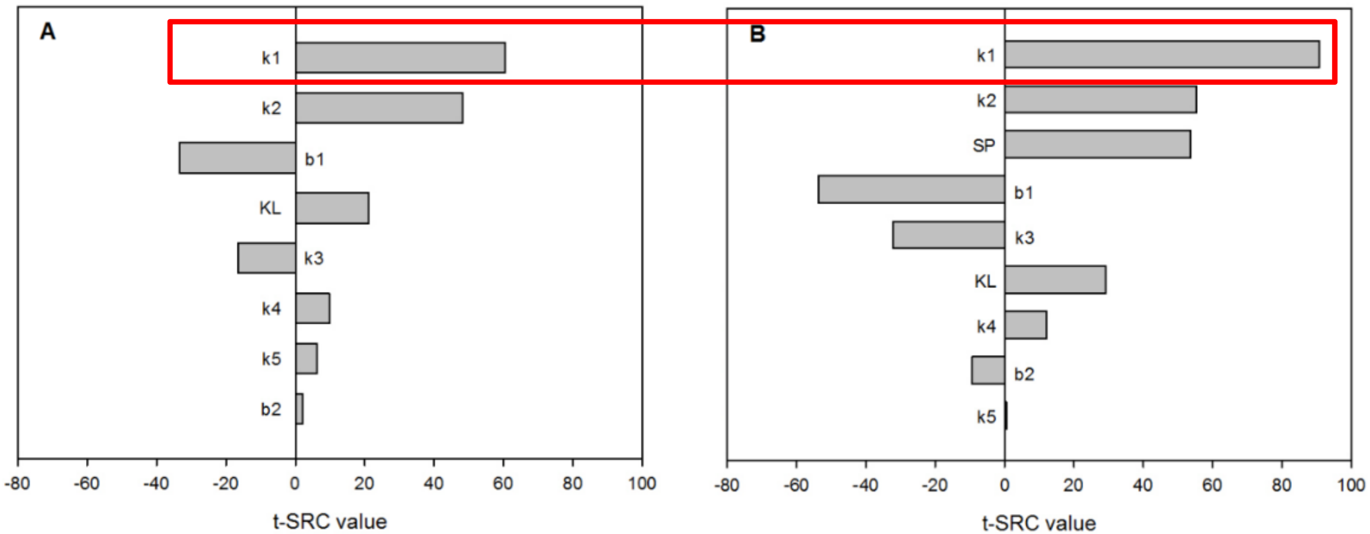


Fig. 3. Experimental (n = 15) and simulated BMP values (A) and the experimental (n = 15) and simulated hydrolysis rate (B) of the anaerobic digestion of miscanthus with the addition of phenolic compounds, represented together with the bisector.

Model testing

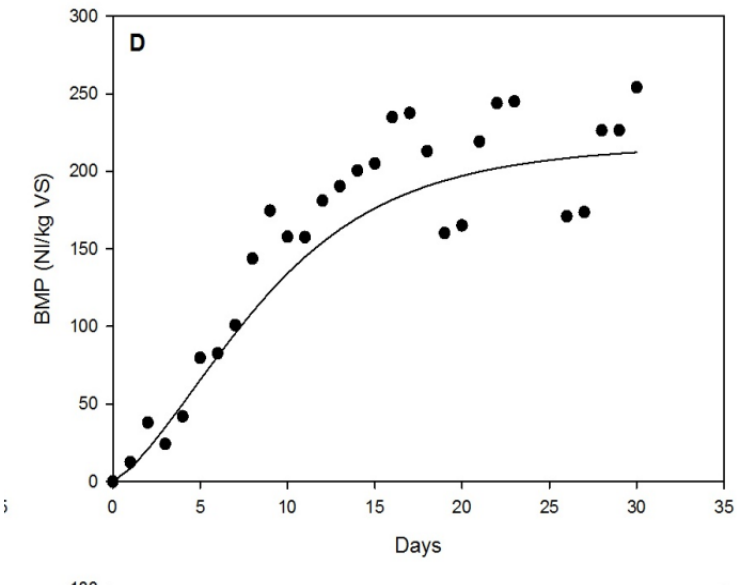
- Global sensitivity analysis $k_1 [VSS] \frac{K_L}{K_L+C_L} \frac{SP+C_P+K_I}{C_P+K_I}$
  - k_1 (hydrolysis) is most important parameter

Without inhibition by C_L With inhibition by C_L



Conclusion

- Succesfull application of a simplified model for batch anaerobic digestion of lignocellulosic biomass
  - Effect of lignin content
  - Effect of phenolic compounds
  - Importance of accuratly describing hydrolysis



GHENT UNIVERSITY

Thanks to the sponsors

led
Laagdrempelige
Expertise- en
Dienstverleningscentra

UNIVERSITEIT GENT
CAMPUS KORTRIJK

fwo

GHENT UNIVERSITY

Some references

- Schroyen, Michel, Vervaeren, H., Vandepitte, H., Van Hulle, S., & Raes, K. (2015). Effect of enzymatic pretreatment of various lignocellulosic substrates on production of phenolic compounds and biomethane potential. BIORESOURCE TECHNOLOGY, 192, 696–702.

- Schroyen, Michel, Vervaeren, H., Raes, K., & Van Hulle, S. (2018). Modelling and simulation of anaerobic digestion of various lignocellulosic substrates in batch reactors: Influence of lignin content and phenolic compounds. BIOCHEMICAL ENGINEERING JOURNAL, 134, 80–87.

- Van Hulle, Stijn, Vesvikar, M., Poutiainen, H. A., & Nopens, I. (2014). Importance of scale and hydrodynamics for modeling anaerobic digester performance. *CHEMICAL ENGINEERING JOURNAL*, *255*, 71–77.

GHENT UNIVERSITY

QUESTIONS?