Development of an Online Tool for the Simulation of the Anaerobic Digestion Process

University of Natural Resources and Applied Life Science, Vienna
Universität für Bodenkultur Wien

Junior Scientist Conference, 19th – 21st April, Vienna

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Anaerobic digestion (AD)

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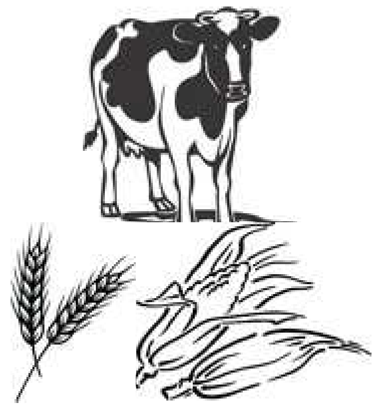

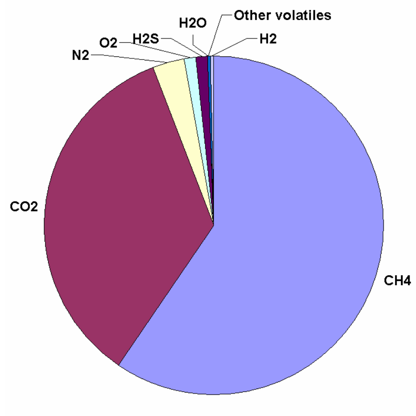

Organic matter → **biogas** + cell material

95% 5%

Multi Step Process

Hydrolysis

Acidogenesis

Acteogenesis

Methanogensis

Anaerobic digestion

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- Characteristics
    - Multi-step process
    - Methane production
    - Low biomass yield

- Advantages
    - Renewable energy
    - Low sludge handle costs
    - Remove pathogen
    - Recycling of nutrients
    - Low energy requirements

- Disadvantages
    - Long retention times
    - Process overload
    - Large reactor
    - Sensitive to environmental changes (pH, Temp)

Anaerobic digestion

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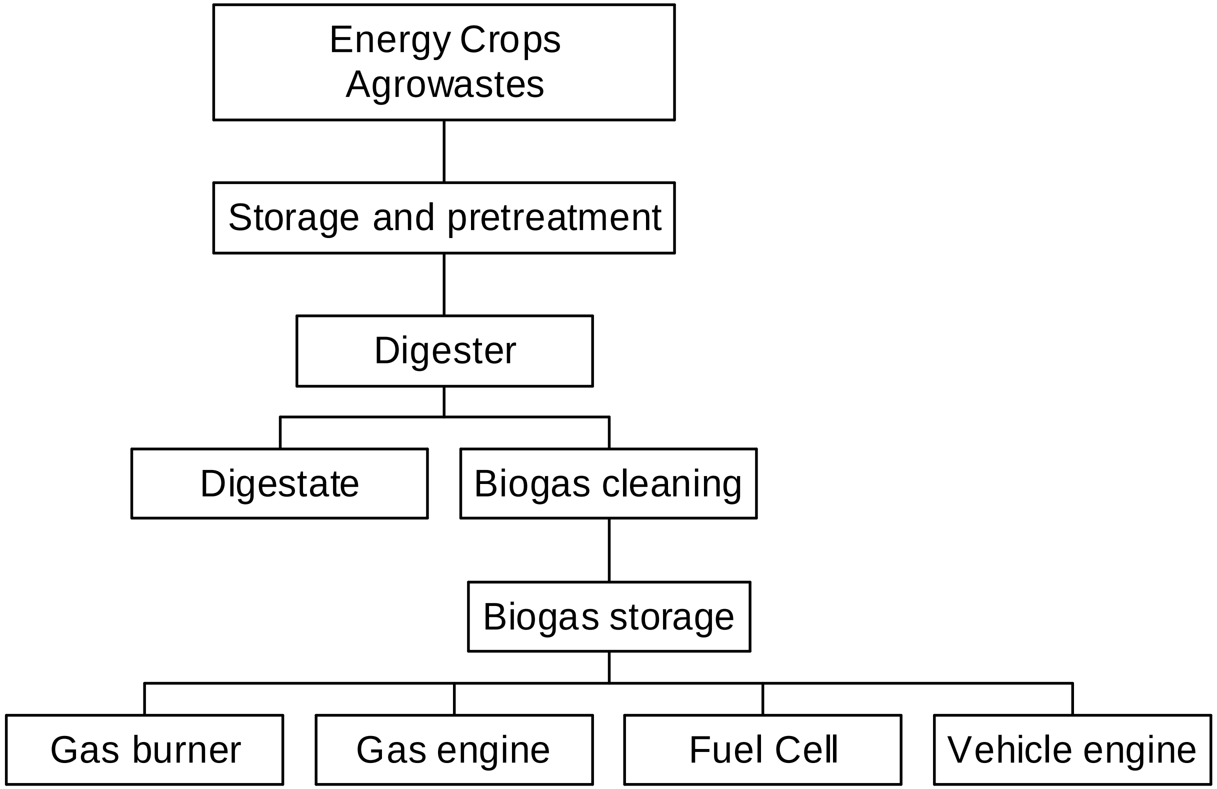

CROPGEN Project

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General

- Project: CROPGEN (Renewable energy from crops and agrowastes)
- Project start: March 2004
  End of project: March 2007
- Project partner: University of Jyväskyla, Metener Ltd., Greenfinch Ltd, Organic Power Ltd., University of Southampton, Instituto de la Grasa, Universita degli Studi di Verona, University of Venice, Wageninen Unversity, University of Natural Resources and Applied Life Science, Vienna
- Objectives: Establishing a sustainable fuel source from biomass, which can be fitted into the actual energy infrastructure and can also supply the hydrogen fuel industry

CROPGEN Project

Modelling and Control

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- Extension and adaptation of an existing AD model

- Virtual laboratory and Decision Support System

- Identification of process-control strategies

Modelling of Anaerobic

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- Hydrolysis controlled Anaerobic Digestion (Jain *et al.*, 1991)
- Model for Dynamic Simulation of Complex Substrates - Focusing on Ammonia inhibition (Angelidaki *et al.*, 1993)
- Simulation Model <Methane> (Vavilin *et al.*, 1993)
- Mathematical Modelling of Anaerobic Digestion (Kiely *et al.*, 1996)
- Comprehensive Model of Anaerobic Bioconversion of Complex substrates (Angelidaki *et al.*, 1998)
- Model for Meso- and Thermophilic Anaerobic Sewage Sludge (Siegrist et al., 2002)
- Anaerobic Digestion Model No.1 (ADM1) (Batstone *et al.*, 2002)

Anaerobic Digestion model No.1 (ADM1)

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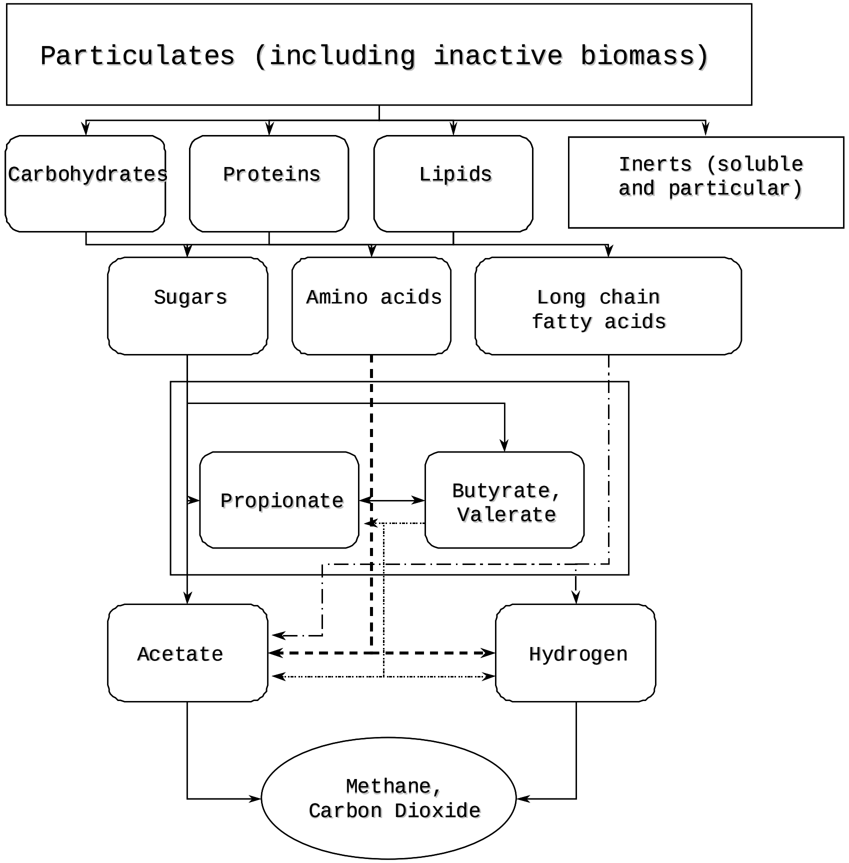

- Model is structured in several steps characterising the biochemical processes
- DAE: 26 dynamic state variables
  19 biochemical kinetic processes
  3 gas-liquid transfer kinetic processes
- DE: 32 dynamic state variables
  6 acid base kinetic processes
- Implementation in a CSTR

Anaerobic Digestion model No.1

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Disintegration:

$$\underbrace{}_{}\frac{dX_c}{dt}=\frac{q_{in}}{V}\left(X_{c,in}-X_c\right)\overbrace{-k_{dis}*X_c}^{\text{Disintegration of complex particulates}}\overbrace{+k_{dec\_Xsu}*X_{su}+k_{dec\_Xaa}*X_{aa}+\ldots}^{\text{Decay of biomass}}$$

Hydrolysis:

$$\frac{dX_{ch}}{dt}=\frac{q_{in}}{V}\left(X_{ch,in}-X_{ch}\right)+f_{ch\_xc}*k_{dis}*X_c-\overbrace{k_{hyd\_ch}*X_{ch}}^{\text{Hydrolysis of carbohydrates}}$$

$$\frac{dX_{pr}}{dt}=\frac{q_{in}}{V}\left(X_{pr,in}-X_{pr}\right)+f_{pr\_xc}*k_{dis}*X_c-k_{hyd\_pr}*X_{pr}$$

$$\frac{dX_{li}}{dt}=\frac{q_{in}}{V}\left(X_{li,in}-X_{li}\right)+f_{li\_xc}*k_{dis}*X_c-k_{hyd\_li}*X_{li}$$

Inert particulates:

$$\frac{dX_I}{dt}=\frac{q_{in}}{V}\left(X_{I,in}-X_I\right)+f_{xI\_xc}*k_{dis}*X_c$$

Anaerobic Digestion model No.1

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Advantages

- First unified model
- Unified Nomenclature and Kinetics
- Basis for further model approaches
- Describes Process Details

Disadvantages

- The model is simplifying the AD process
- No validation of biological parameters
- No information on the effect of inhibitory compounds
- No information on the effect on kinetics in different temperature ranges
- Requirement of detailed substrate definition
- The COD flow is rather complex

Adaptation of the ADM1

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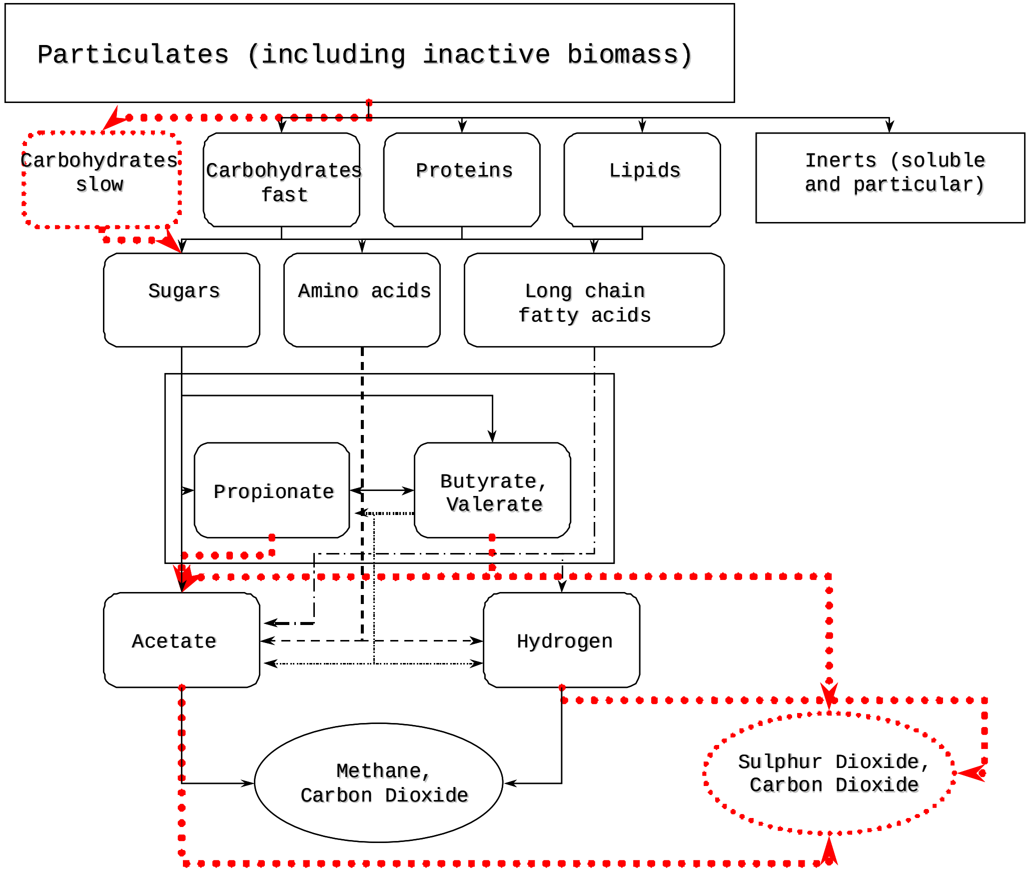

Adaptation of the ADM1

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cropgen

Additional Differential equation – Additional Hydrolysis rate:

$$\frac{dX_{ch\_s}}{dt} = \frac{q_{in}}{V}\left(X_{ch\_s,in} - X_{ch\_s}\right) + f_{ch\_s\_xc} * k_{dis} * X_c - k_{hyd\_ch\_s} * X_{ch\_s}$$

Excerpt Differential equations – Sulphate reduction process:

$$\frac{dS_{ac}}{dt} = \frac{q_{in}}{V_{liq}}\left(S_{ac,in} - S_{ac}\right) + (1 - Y_{su}) f_{ac,su}\rho_5 + (1 - Y_{aa}) f_{ac,aa}\rho_6 + (1 - Y_{fa})0.7\rho_7 +$$
$$(1 - Y_{c4})0.31\rho_8 + (1 - Y_{c4})0.8\rho_9 + (1 - Y_{pro})0.57\rho_{10} - \rho_{11} + (1 - Y_{x5})0.8\rho_{20} + (1 - Y_{x6})0.57\rho_{21} - \rho_{22}$$

$$\frac{dS_{pro}}{dt} = \frac{q_{in}}{V_{liq}}\left(S_{pro,in} - S_{pro}\right) + (1 - Y_{su}) f_{pro,su}\rho_5 + (1 - Y_{aa}) f_{pro,aa}\rho_6 + (1 - Y_{c4})0.54\rho_8 - \rho_{10} - \rho_{21}$$

$$\frac{dS_{bu}}{dt} = \frac{q_{in}}{V_{liq}}\left(S_{bu,in} - S_{bu}\right) + (1 - Y_{su}) f_{bu,su}\rho_5 + (1 - Y_{aa}) f_{bu,aa}\rho_6 - \rho_9 - \rho_{20}$$

$$\frac{dS_{h2}}{dt} = \frac{q_{in}}{V_{liq}}\left(S_{h2,in} - S_{h2}\right) + \rho \ldots\ldots\ldots\ldots - \rho_{23}$$

$$\rho_{20} = \frac{k_{m,so4bu} \cdot S_{bu}}{K_{s,so4bu} + S_{bu}} \cdot \frac{S_{so4}^{2-}}{K_{so4bu} + S_{so4}^{2-}} \cdot X_5 \cdot I_{pH,13} \cdot I_{h2s,x5}$$

Adaptation of the ADM1

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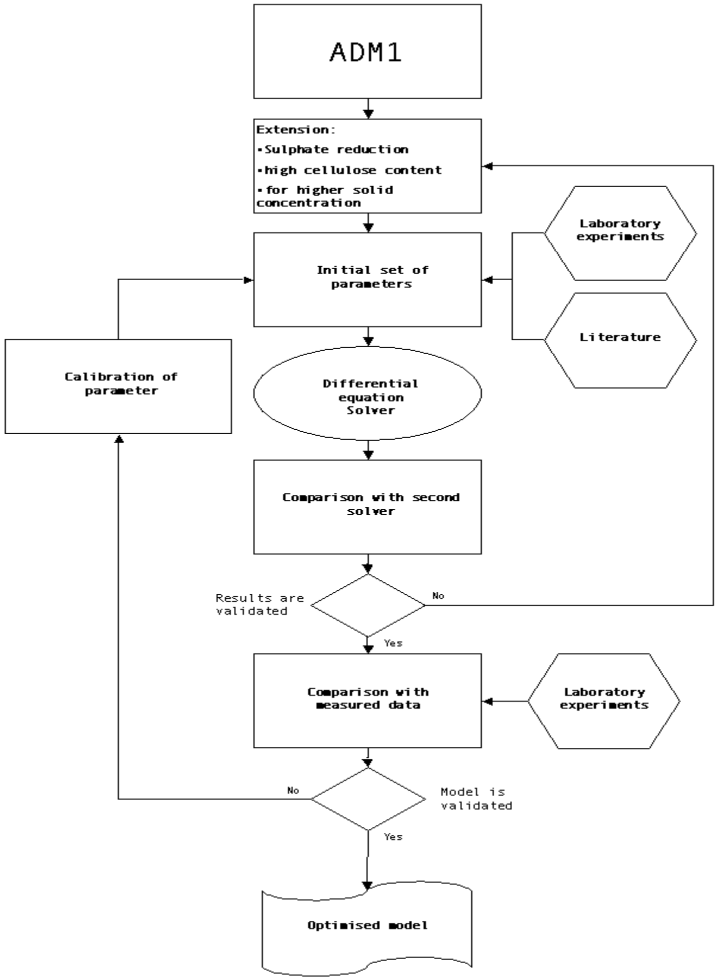

Adaptation of the ADM1

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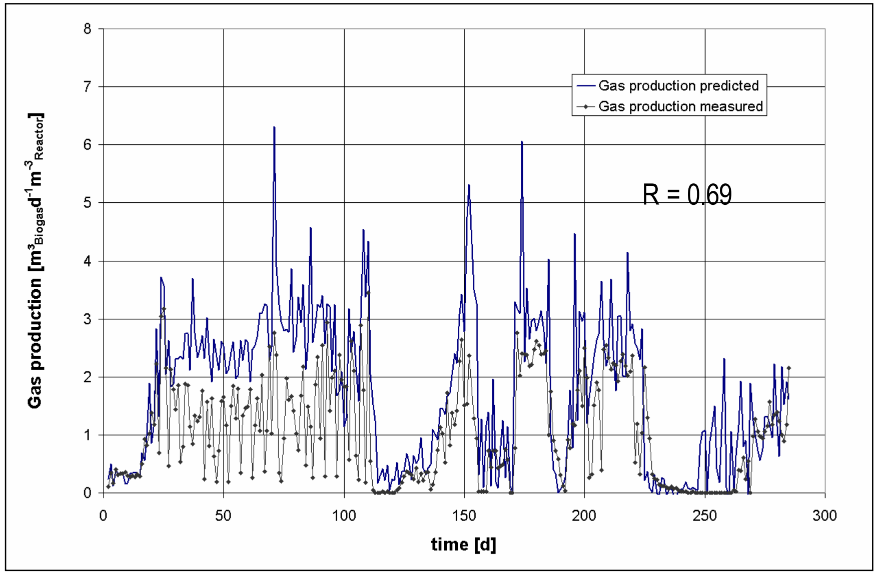
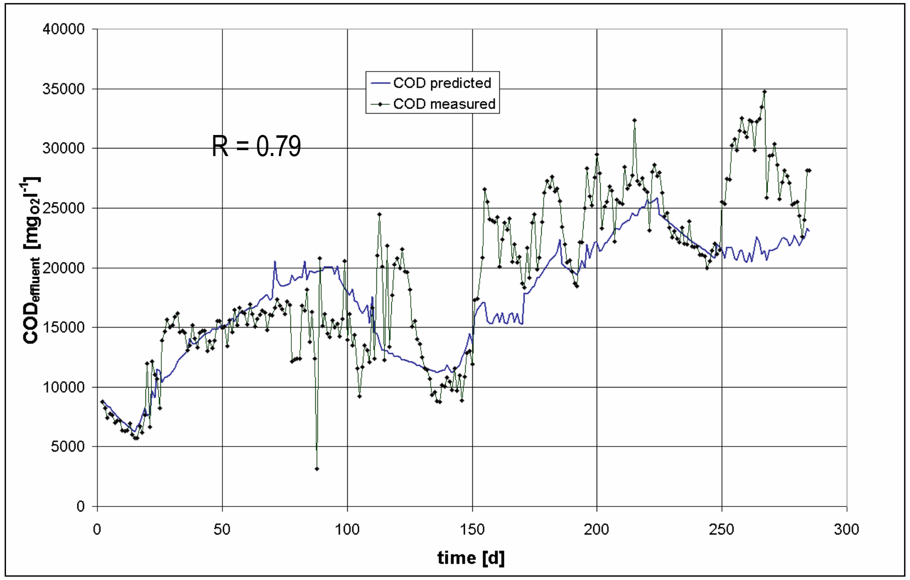
Model results





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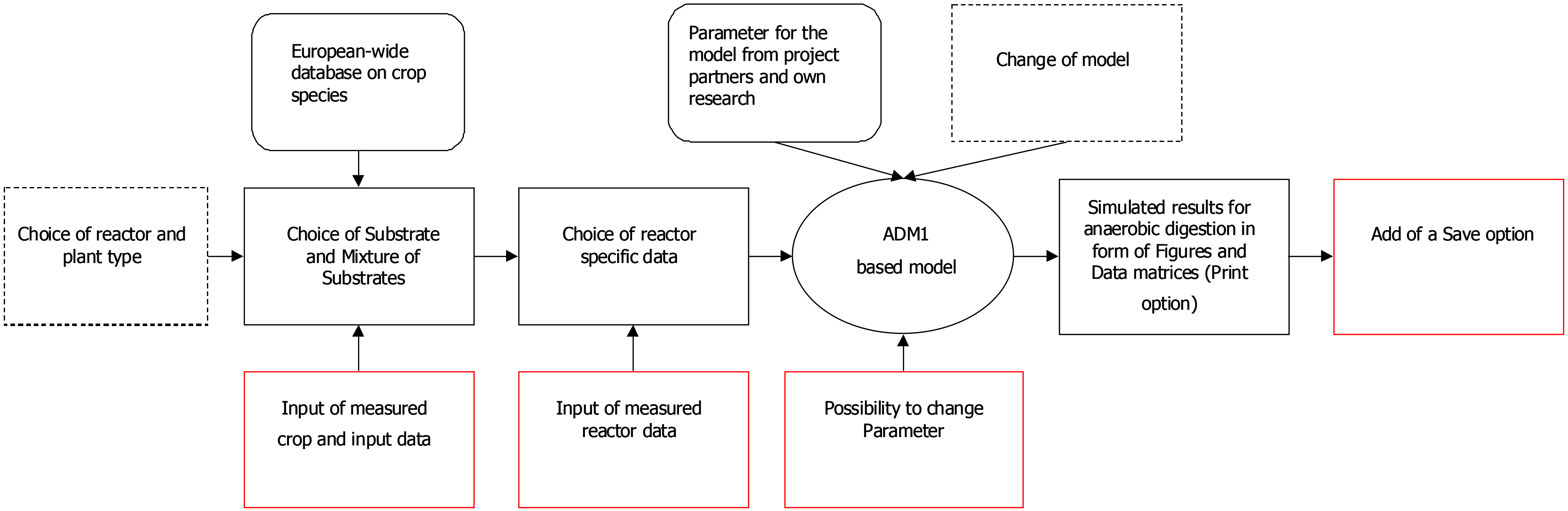
Structure



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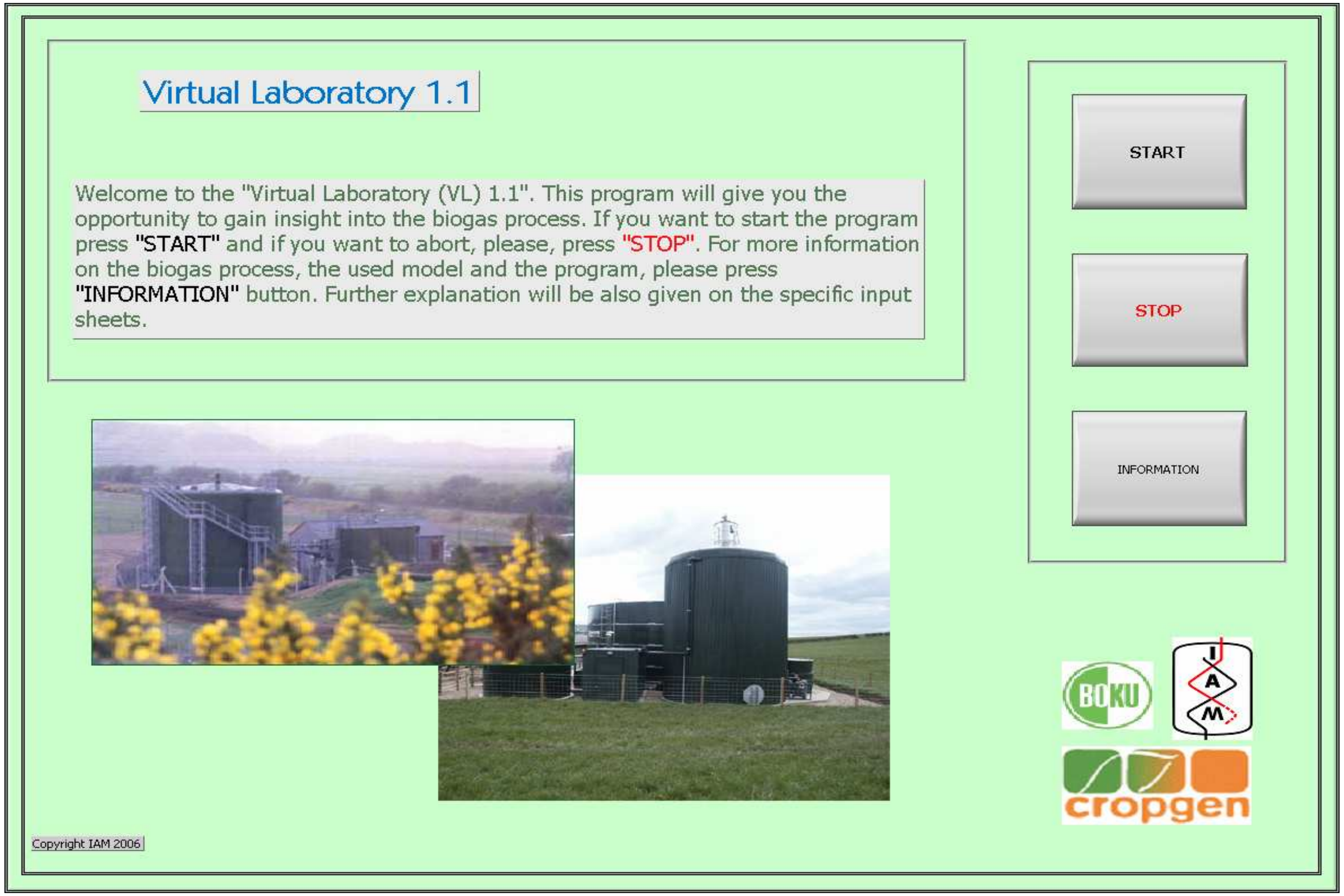
Screenshot 1



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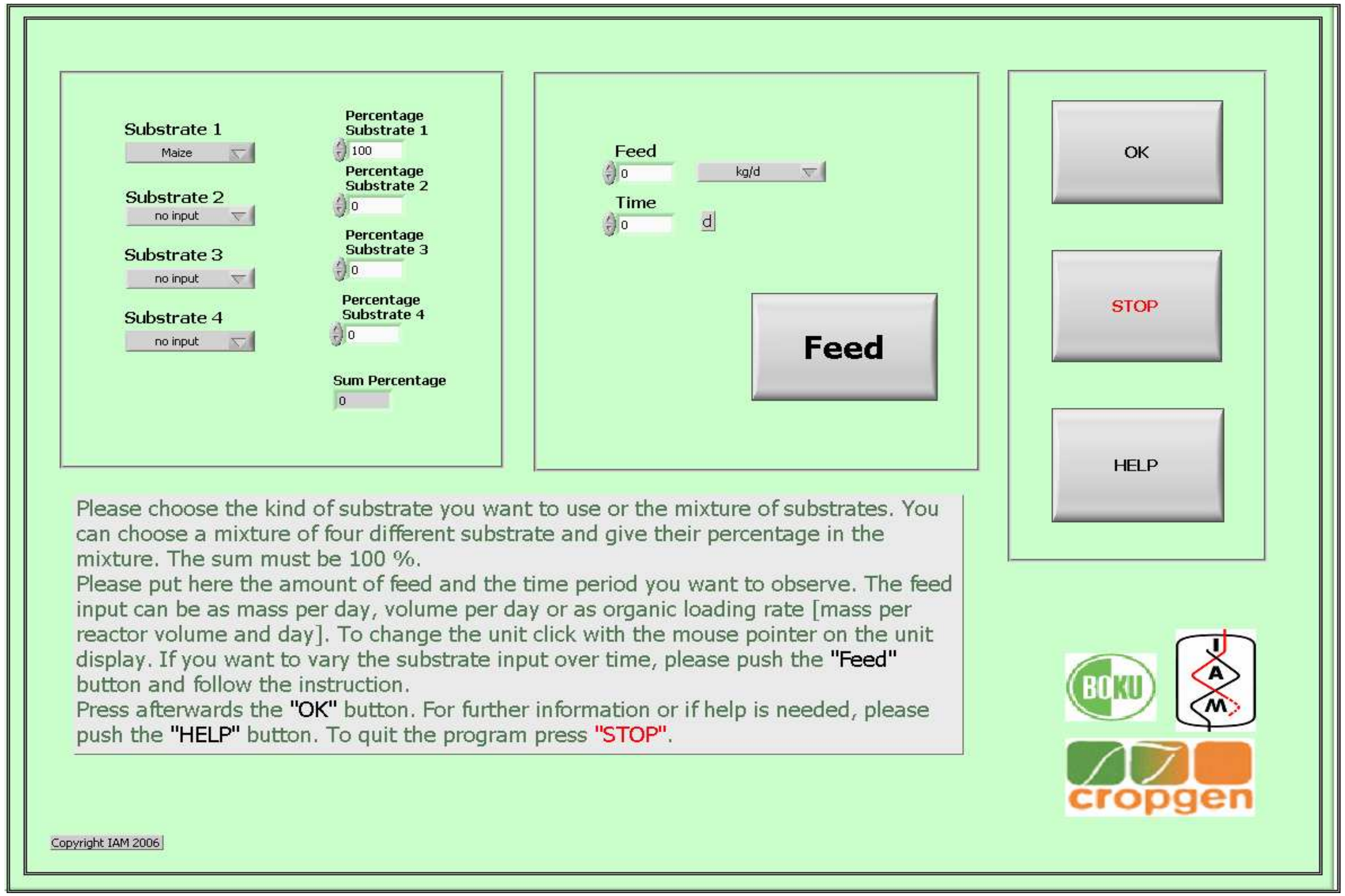
Screenshot 2



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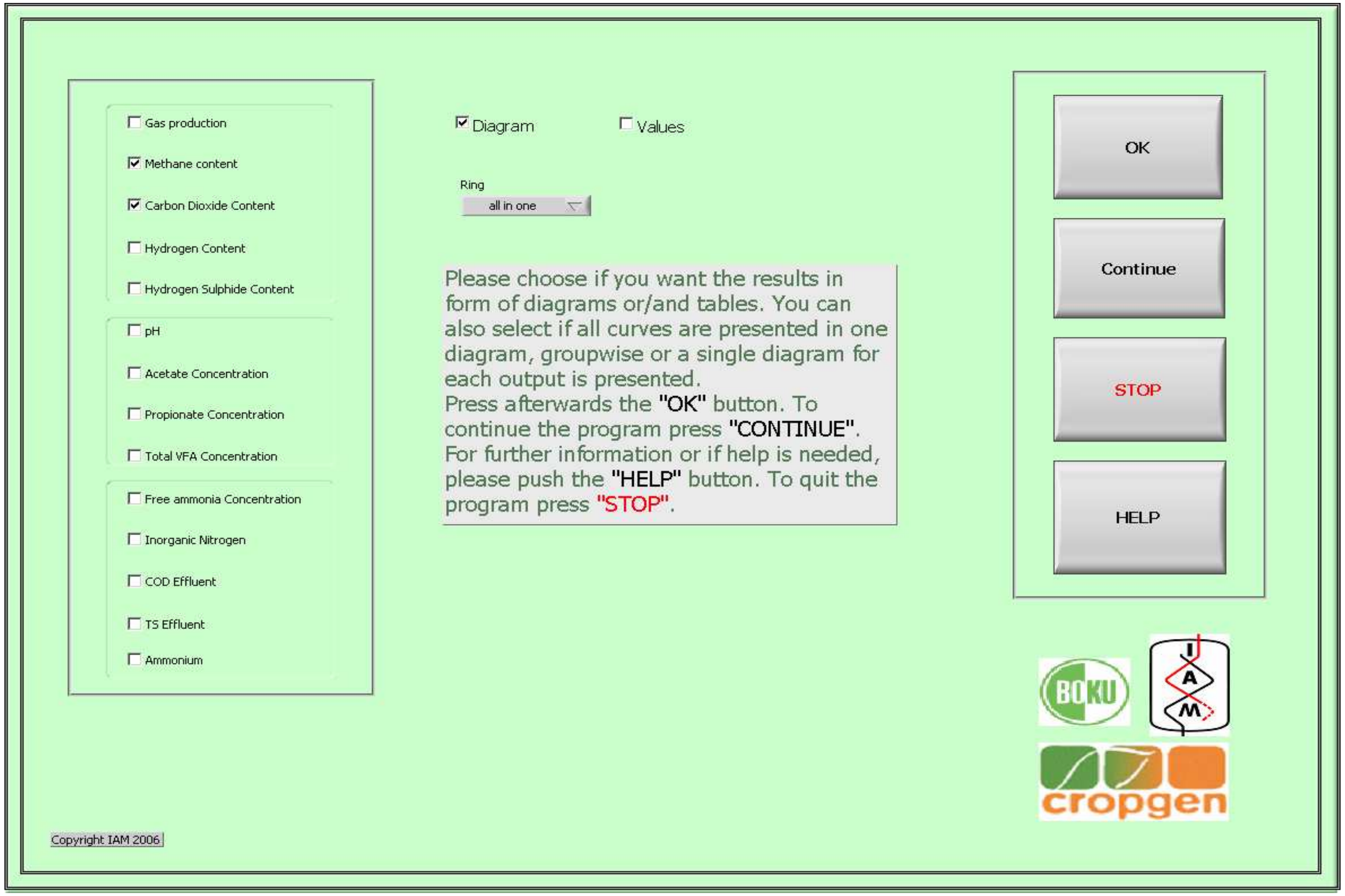
Screenshot 3



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Screenshot 4

Summary & Conclusion

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- AD of Biomass as sustainable fuel source
- Cost optimisation through improved process control & monitoring
- Complex process
- Adaptation of an existing AD model
  - Addition of a second hydrolysis rate for carbohydrates
  - Implementation of the sulphate reduction process
- Development of an Online Tool
  - CROPGEN Homepage

  http://www.cropgen.soton.ac.uk/
- Mathematical model as basis for a control tool

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Thank you for your attention.

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