

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



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Universität für Bodenkultur Wien



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

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- CROPGEN Project
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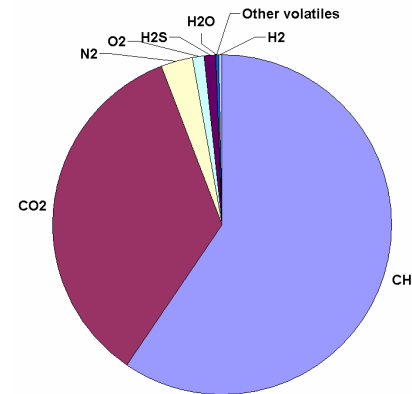
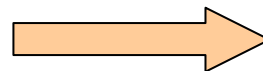
Anaerobic digestion (AD)



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Organic matter



biogas + cell material

95%

5%

Multi Step Process

Hydrolysis

Acidogenesis

Acteogenesis

Methanogenesis

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

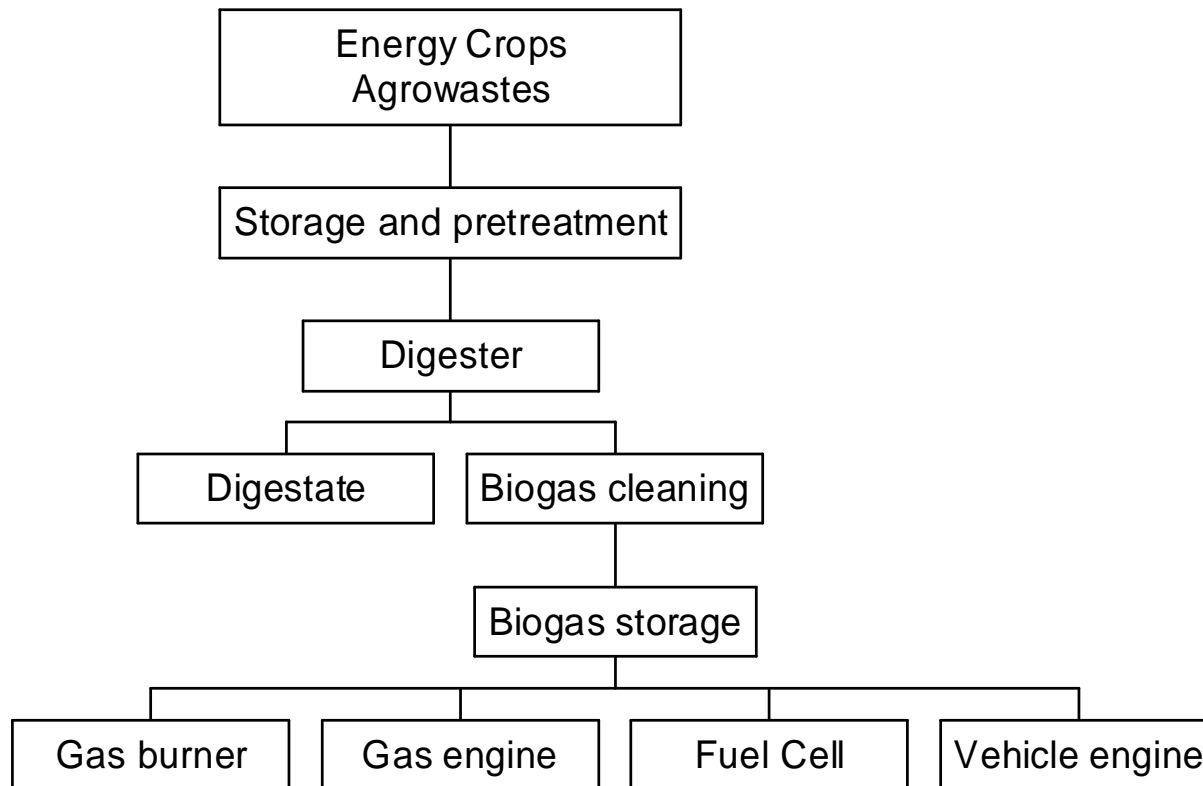
•Disadvantages

- 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 Jyväskylä, Metener Ltd., Greenfinch Ltd, Organic Power Ltd., University of Southampton, Instituto de la Grasa, Università degli Studi di Verona, University of Venice, Wageninen University, 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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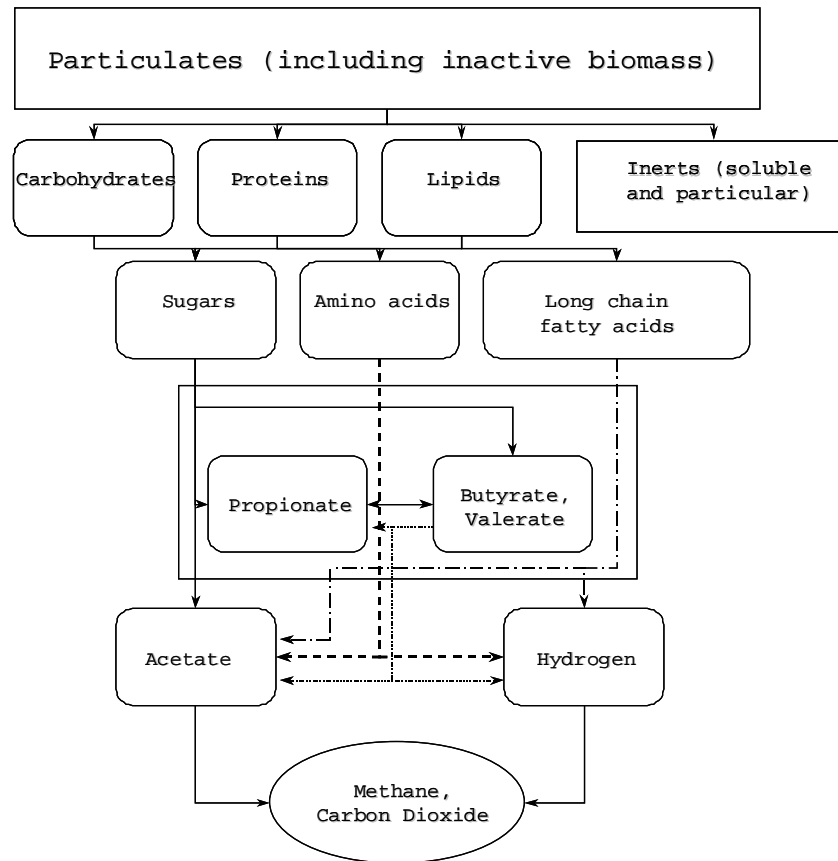


- Hydrolysis controlled Anaerobic Digestion (Jain *et al.*, 1991)
- Model for Dynamic Simulation of Complex Substrates - Focusing on Ammonia inhibition (Angelidaki *et al.*, 1993)
- Simulation Model <Methane> (Vavilin *et al.*, 1993)
- Mathematical Modelling of Anaerobic Digestion (Kiely *et al.*, 1996)
- 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: Disintegration of complex
particulates Decay of biomass

$$\frac{dX_c}{dt} = \frac{q_{in}}{V} (X_{c,in} - X_c) - k_{dis} * X_c + k_{dec_Xsu} * X_{su} + k_{dec_Xaa} * X_{aa} + \dots$$

Hydrolysis: Hydrolysis of carbohydrates

$$\frac{dX_{ch}}{dt} = \frac{q_{in}}{V} (X_{ch,in} - X_{ch}) + f_{ch_xc} * k_{dis} * X_c - k_{hyd_ch} * X_{ch}$$

$$\frac{dX_{pr}}{dt} = \frac{q_{in}}{V} (X_{pr,in} - X_{pr}) + f_{pr_xc} * k_{dis} * X_c - k_{hyd_pr} * X_{pr}$$

$$\frac{dX_{li}}{dt} = \frac{q_{in}}{V} (X_{li,in} - X_{li}) + f_{li_xc} * k_{dis} * X_c - k_{hyd_li} * X_{li}$$

Inert particulates:

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

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

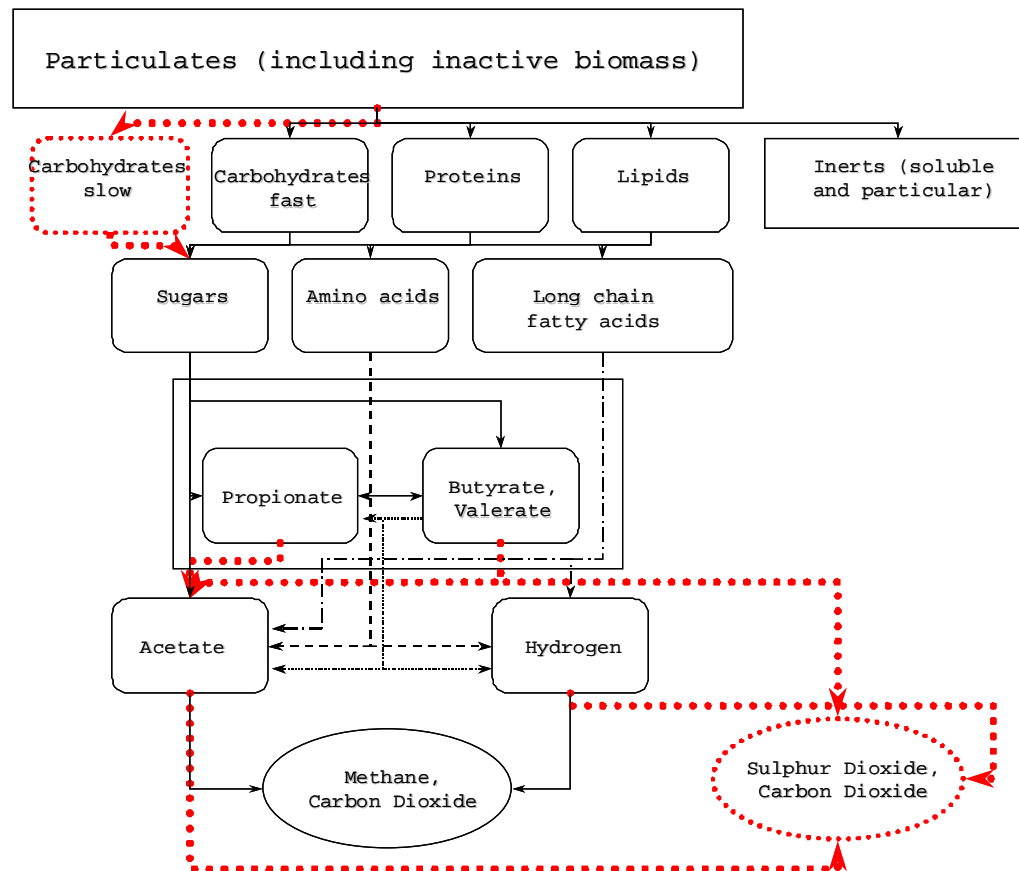
Disadvantages

- 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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Additional Differential equation – Additional Hydrolysis rate:

$$\frac{dX_{ch_s}}{dt} = \frac{q_{in}}{V} (X_{ch_s,in} - X_{ch_s}) + f_{ch_s_xc} * k_{dis} * X_c - k_{hyd_ch_s} * X_{ch_s}$$

Excerpt Differential equations – Sulphate reduction process:

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

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

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

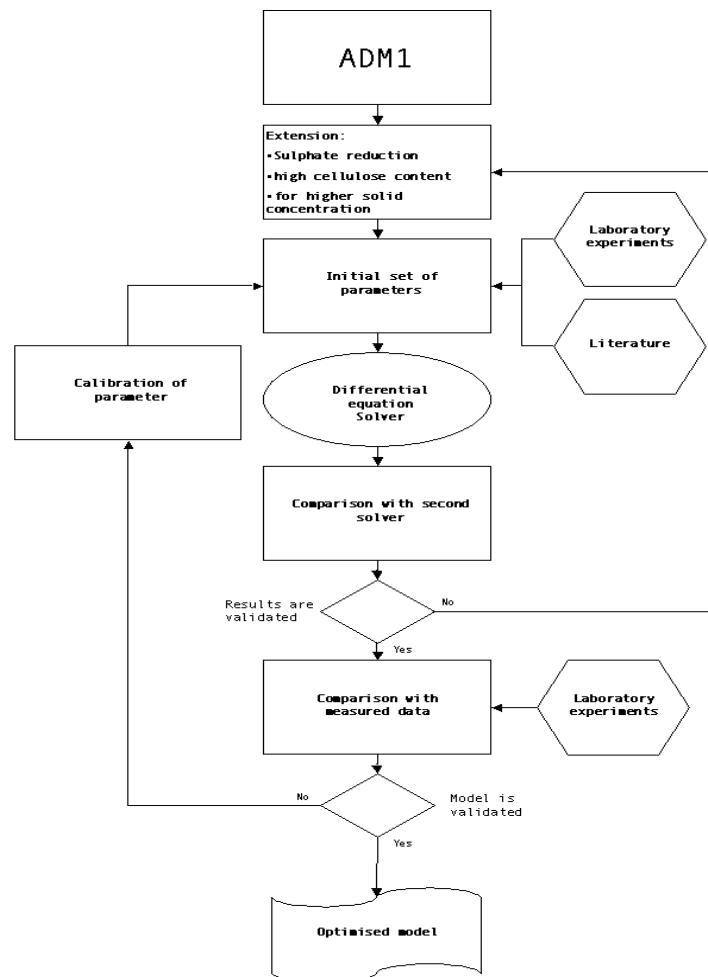
$$\frac{dS_{h2}}{dt} = \frac{q_{in}}{V_{liq}} (S_{h2,in} - S_{h2}) + \rho_{23}$$

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

Adaptation of the ADM1



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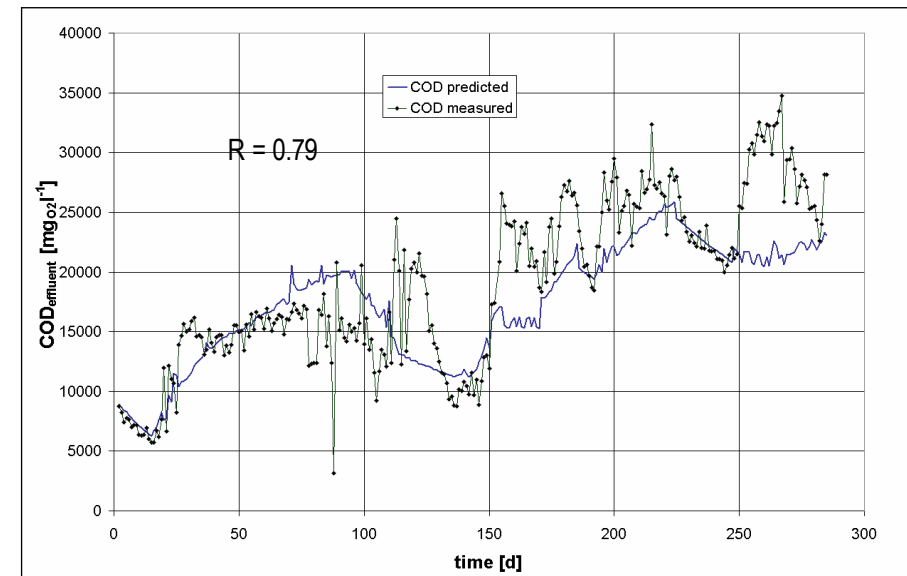
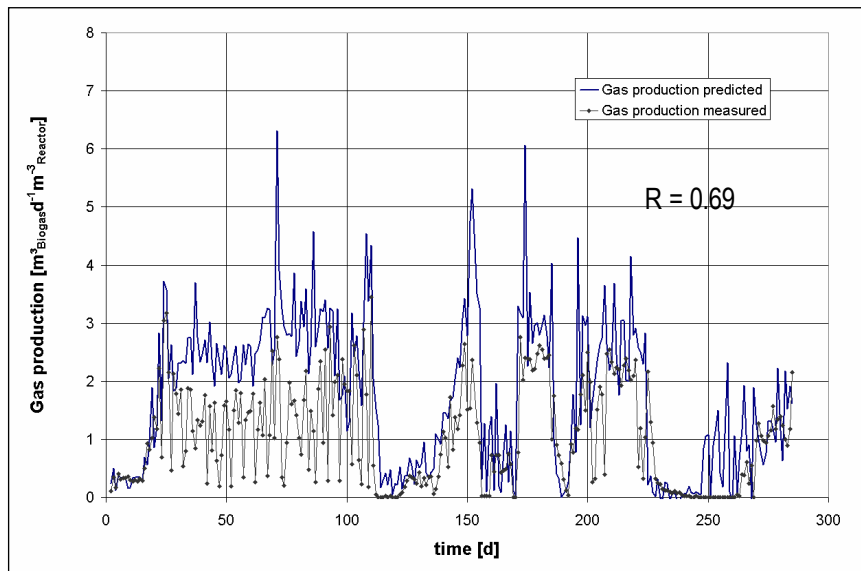
Adaptation of the ADM1



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Model results



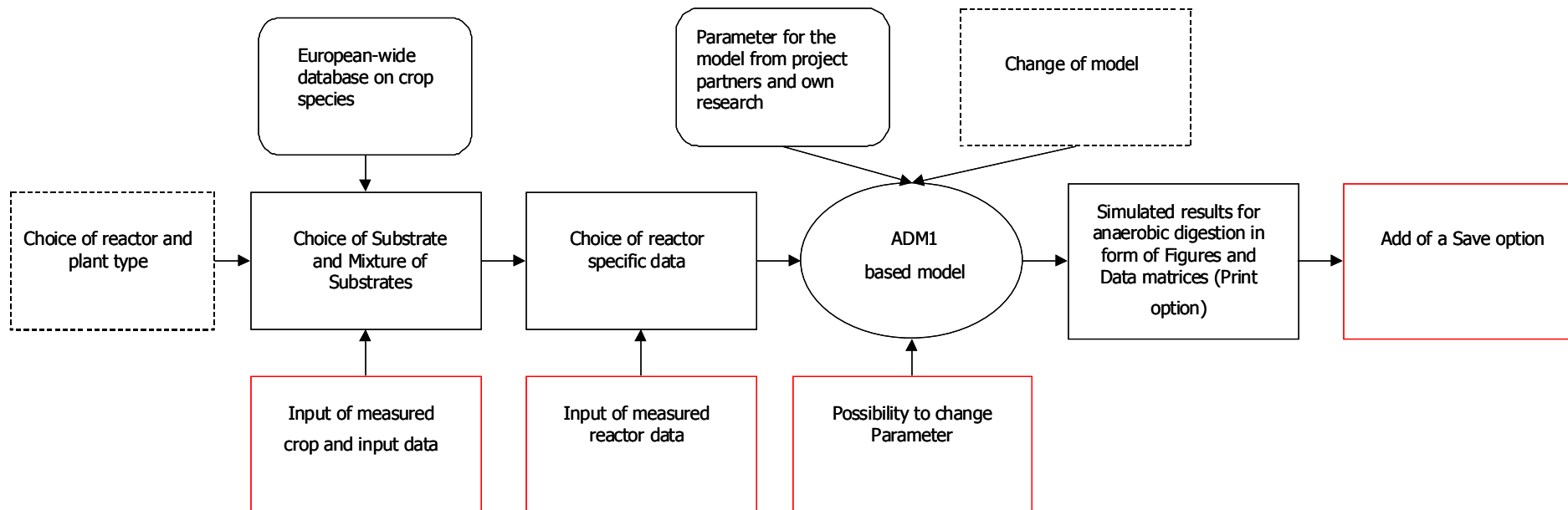
Virtual Laboratory



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Structure



Virtual Laboratory




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Screenshot 1

Virtual Laboratory 1.1

Welcome to the "Virtual Laboratory (VL) 1.1". This program will give you the opportunity to gain insight into the biogas process. If you want to start the program press "START" and if you want to abort, please, press "STOP". For more information on the biogas process, the used model and the program, please press "INFORMATION" button. Further explanation will be also given on the specific input sheets.




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START

STOP

INFORMATION



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Screenshot 2

The screenshot displays a virtual laboratory interface with the following components:

- Substrate Selection Panel:** Four dropdown menus for Substrate 1 (Maize), Substrate 2 (no input), Substrate 3 (no input), and Substrate 4 (no input). To the right, percentage input fields for each substrate are set to 0, except for Substrate 1 which is set to 100. A 'Sum Percentage' field shows 0.
- Feed Input Panel:** A 'Feed' input field set to 0 with a unit dropdown menu set to 'kg/d'. A 'Time' input field set to 0 with a unit dropdown menu set to 'd'. A large 'Feed' button is positioned below these inputs.
- Control Panel:** Three buttons labeled 'OK', 'STOP', and 'HELP' are arranged vertically on the right side.
- Instructional Text:** A text box at the bottom left provides instructions: "Please choose the kind of substrate you want to use or the mixture of substrates. You can choose a mixture of four different substrate and give their percentage in the mixture. The sum must be 100 %. Please put here the amount of feed and the time period you want to observe. The feed input can be as mass per day, volume per day or as organic loading rate [mass per reactor volume and day]. To change the unit click with the mouse pointer on the unit display. If you want to vary the substrate input over time, please push the 'Feed' button and follow the instruction. Press afterwards the 'OK' button. For further information or if help is needed, please push the 'HELP' button. To quit the program press 'STOP'."
- Logos:** BOKU and cropgen logos are located at the bottom right of the interface.
- Copyright:** Copyright IAM 2006 is noted at the bottom left.

Virtual Laboratory



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Screenshot 3

The screenshot shows a configuration window with a light green background. On the left, there is a list of checkboxes for various data outputs: Gas production, Methane content (checked), Carbon Dioxide Content (checked), Hydrogen Content, Hydrogen Sulphide Content, pH, Acetate Concentration, Propionate Concentration, Total VFA Concentration, Free ammonia Concentration, Inorganic Nitrogen, COD Effluent, TS Effluent, and Ammonium. In the center, there are radio buttons for 'Diagram' (checked) and 'Values', and a dropdown menu labeled 'Ring' with 'all in one' selected. A text box in the center contains instructions: 'Please choose if you want the results in form of diagrams or/and tables. You can also select if all curves are presented in one diagram, groupwise or a single diagram for each output is presented. Press afterwards the "OK" button. To continue the program press "CONTINUE". For further information or if help is needed, please push the "HELP" button. To quit the program press "STOP".' On the right, there are four buttons: 'OK', 'Continue', 'STOP' (in red), and 'HELP'. At the bottom right, there are logos for BOKU and cropgen, along with a DNA helix icon containing the letters J, A, and M. A copyright notice 'Copyright IAM 2006' is visible in the bottom left corner of the window.

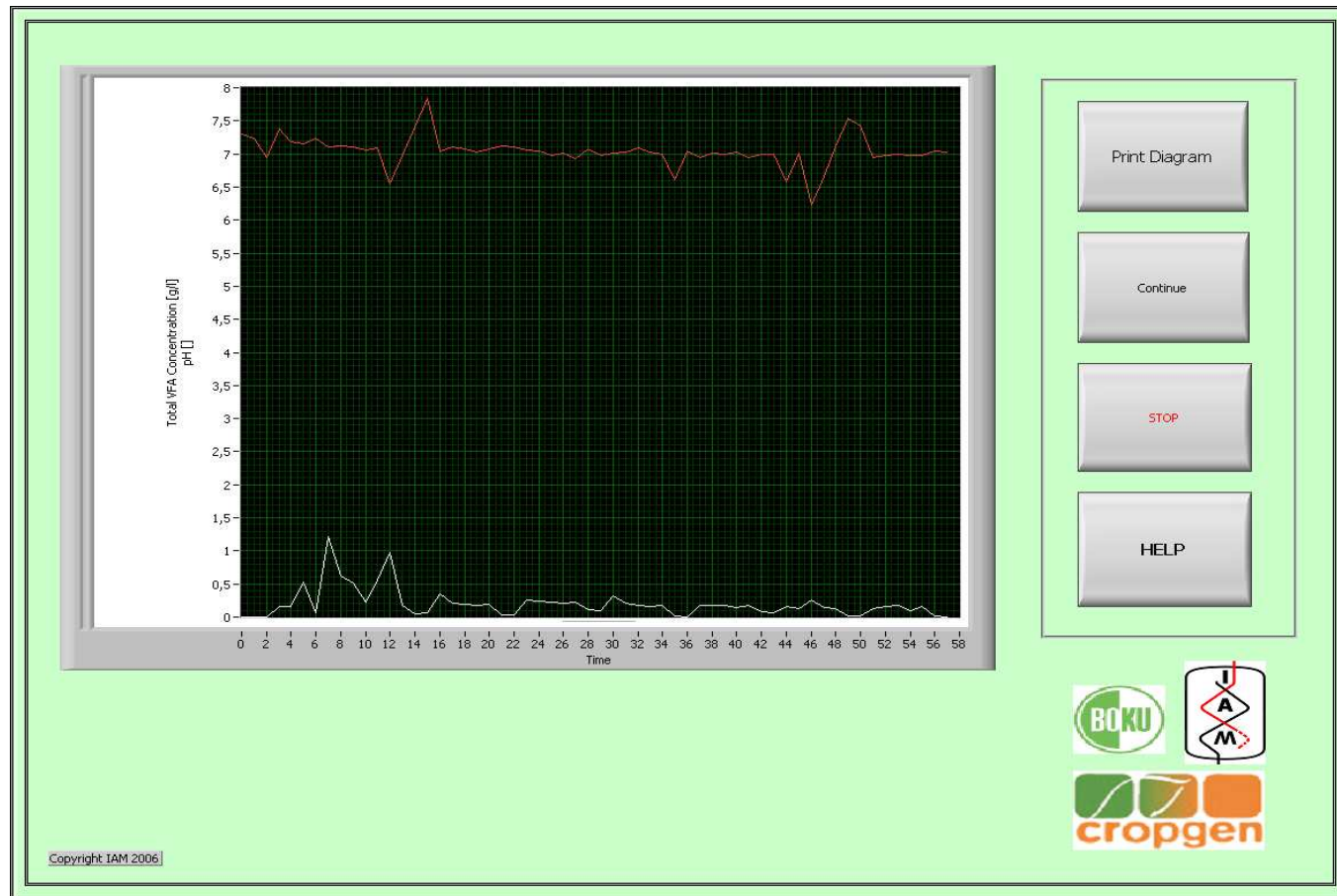


Virtual Laboratory



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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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