Modelling and Simulating Energy Conversion Processes using Modelica

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Abstract: The paper describes the ongoing work on modeling and simulation of energy conversion processes. The models have been implemented in Modelica language and simulated in Dymola environment. The studied processes are a biomass fired Circulating Fluidized Bed (CFB) boiler and an anaerobic digester for biogas production. The models were validated towards real process data. The models have been running on-line and off-line respectively. The aim of the paper is to demonstrate the potentials and limitations of the simulation approach proposed as well as highlight the possibility of reusing the designed libraries in other energy conversion systems. The proposed approach has shown acceptable results for process diagnostics and can be used for the study of other energy systems.

Keywords: Dynamic simulation, Modelica, Energy conversion, CFB boiler, biogas, diagnostics.

1. INTRODUCTION

Due to the demanding environmental constraints, efforts have been in recent years focused on improving the efficiency of energy conversion processes. Biomass as renewable energy source has become very popular to substitute the scarce fossil fuels and contribute to the reduction of green-house gases. Biomass is used as fuel in many energy conversion systems; it can be directly fired, co-fired or gasified to produce both heat and electricity. Biomass can as well be converted to be used as a transportation fuel. One of the drawbacks of biomass as a renewable energy source is its heterogenic chemical composition. This characteristic of biomass influences the conversion system efficiency to great extent.

Dynamic simulation tools are especially useful for fault detection as well as to determine optimal control strategies as described in Venkatasubramanian et al. (2003, a, b, c). The control requirements for biomass to energy processes might become challenging due to the varying composition of the raw material. Dynamic models are useful for fault detection, plant design and operator training; to instruct the plant operators about conventional and emergency procedures, as well as to help them in determining the parameters for optimal plant operation. The combination of physical models with statistical models is an extended approach for decision support as in Avelin et al. (2009). The use of dynamic simulation models to determine maintenance operation has earned popularity in recent years as in Ciarapica et al. (2006).

Energy conversion systems models are usually complex models which require a high structured programming language. Generally dynamic models are preferred in order to reach a deeper understanding of the process. Fritzon (2007) points out Modelica as a straightforward object oriented language developed for modelling of large physical systems. Dymola is an engineering simulation tool compatible with Modelica language which provides with the interface to develop the system model. Dymola includes several Modelica libraries for different domains, electrical, hydraulic, thermodynamic, chemical systems among others. A thermo power library has been developed by Otter et al. (2001). Several works where Modelica libraries for power plants as in Casella et al. (2005) and other energy conversion systems as in Salogni et al. (2010) have been also developed. In Casella et al. (2007) a dynamic model of a biomass-fired-power-plant is presented. In Casella et al. (2012) a dynamic model of a gasifier is implemented in Modelica. However, this wide range of libraries is not always suitable for the specific application that should be addressed

In this work, Modelica component libraries with process components for a biomass fired CFB boiler and an anaerobic digester for biogas production were created. Earlier we also have built a Modelica model for a CFB black liquor gasification process. The component models are represented graphically and stored in the designed Modelica libraries. Once the component models have been defined the physical connection can be established. The models have been validated towards process data and have been used for fault detection and diagnostics.

The purpose of this work is to demonstrate the potentials and limitations of the dynamic simulation tool used as well as highlight the possibility of reusing the designed model libraries. This article starts with a brief description of the models. The model validation based on process data is presented. Finally some concluding remarks and description of future plans are highlighted.

2. APPROACH DESCRIPTION

The dynamic simulation approach is depicted in Fig. 1.
The common phenomena for all three proposed energy conversion processes are presented in Fig. 1. The systematic approach works as following:

- The physical models are implemented in the acausal programming language Modelica.
- Process data from the distributed control system (DCS) is used for validation.
- The proposed simulation tool can be used off-line as well as on-line.
- A comparison between measured values and simulation results for a specific process variable is carried out in order to determine an optimal control strategy or diagnose process upsets.

An on-line application of the proposed dynamic simulation approach has been used in the simulation of a CFB boiler. Here the connection between the DCS and the simulation model is established with Simulink, allowing better control of the signal processing between simulation and the process database. On the other hand the anaerobic digester model has been running off-line. The input signal into the digester block is generated using the Modelica standard library block “TimeTable” which receives a table of time and values and generates them into an output signal (can be discontinuous if the same time is given two values).

### 2.1 Boiler

The CFB boiler model includes the combustion section as well as water/steam and exhaust gas train. The model is validated towards real plant data and is capable of successfully predict operation performance. An exhaustive description of this model can be found in Sandberg et al. (2011). During 2010 and 2011 the model was used on-line at Mälarenenergi AB (local power and heat generation plant) for diagnostic purposes.

Biofuel, air, sand and material from the Intrex are fed to the boiler, while ash and flue gas including sand and dust is leaving the bed. Also heat is transferred to the steam system in the boiler, in the separators (cyclones), in the Intrex and in a series of heat exchangers in the exhaust gas train. Temperature, gas composition and flow rates are measured all the way through the boiler and exhaust gas train and in the steam system. These measurements are then compared to the values predicted from the simulation using the same input data. This includes fuel flow, fuel composition, air flow and feed water flow to the steam dome. Unfortunately the fuel composition cannot be measured; if moisture content varies the impact will be significant.

The equations used are primarily stoichiometric calculations of how the biomass is converted through combustion, giving adiabatic temperature and cooling through heat transfer and through transport of material from the boiler combustion zone. The mass in the bed inventory by time is given from:

$$\frac{\partial m_{\text{inventory}}}{\partial t} = \sum m_{i,\text{in}} - \sum m_{i,\text{out}}$$  \hspace{1cm} (1)

where $m_{i,\text{in}}$ is the mass input flow of each single component of the composition vector $i = \{\text{C,H,O,N,CO}_2,\text{H}_2\text{O,NO}_2,\text{ash}\}$ and $m_{i,\text{out}}$ is the corresponding output flow. The change in concentration of each component is given by $c_i$ in the bed inventory:

$$\frac{\partial c_i}{\partial t} = \left(\sum (c_i \cdot m_j)_{\text{in}} - \sum (c_i \cdot m_k)_{\text{out}}\right) / m_{\text{inv.}}$$ \hspace{1cm} (2)

where $j$ are all incoming flows and $k$ all outgoing flows of the inventories. Except the bed inventory we also have one
inventory for the Intrex and one for the steam system. The steam system has only water and steam components, while the Intrex has the same components as the bed. The temperature $T_{\text{inventory}}$ in the inventory is calculated from the energy balance:

$$\frac{\partial T_{\text{inventory}}}{\partial t} = \left( \left( \sum T_i \cdot c_{p_i} \cdot m_{i_{\text{in}}} \right) - \left( \sum T_i \cdot k \cdot c_{p_i} \cdot c_{i_{\text{m}}} \right) \right) / \left( m_{\text{inventory}} \cdot (\sum c_{p_i} \cdot c_{p_i}) \right)$$

(3)

Here $\Delta H$ (enthalpy) is the energy released during combustion and $U$ is the overall heat transfer coefficient, $A$ is the heat exchanger area and $T_{\text{outside}}$ the temperature at the other side of the heat exchanger surface (steam temperature vs. exhaust gas temperature). $c_{p_i}$ is the heat capacity for each component $i$.

The correlations describing the change in each single component is also included in the model. Carbon, C, in the biomass is combusted to CO$_2$, and the hydrogen is forming H$_2$O. Oxygen, O, in the fuel is used for the combustion aside of the oxygen in the air. N, in the fuel is assumed oxidized to NO$_2$ partly, as a function of oxygen surplus and temperature. Separation of sand is performed in cyclones and cooling in heat exchangers with gas to gas, gas to steam or gas to water transfer. We have not included inventories in the heat exchangers as the residence time is very short.

2.2 Other energy conversion processes

The anaerobic digester model describes the process using kinetic equations and mass balances. The main block in the model is the digester block consisting of 22 equations. The model assumes the hydrolysis as the limiting rate or limiting step of the process and describes the hydrolysis using first-order kinetics. The model is validated against process data from a full-scale biogas plant, Växtkraft in Västerås, which uses organic municipal solid waste, grease trap sludge and silage as substrate.

For high temperature gasification we have similar reactions to the anaerobic digester, but a process configuration being very similar to the boiler application.

The energy and material balances are principally modelled in the same way for the anaerobic digestion and the boiler. In the boiler model the combustion is handled by the conversion of C and H into CO$_2$ and H$_2$O while we have a more complex situation for the anaerobic digestion. Still, the final products are mainly CO$_2$, H$_2$O and CH$_4$ from the anaerobic digestion.

This can be modelled as an extension of eq (2):

$$\frac{\partial c_i}{\partial t} = \left( \left( \sum (c_i \cdot m_{i_{\text{in}}}) - k \cdot [c_i]^a \right) - \sum (c_i \cdot m_{k_{\text{out}}}) \right) / m_{\text{inv.}}$$

(4)

where $k$ is a reaction constant and $a$ an exponent giving the non-linearity of the conversion. For components being removed $c_i$ is decreasing while for those being created it is increasing. This is for a certain volume element that can be the complete reactor or a smaller part of it.

3. MODEL VALIDATION AND RESULTS

The boiler simulation model was verified towards process data. In Table 1 we can see one set of data:

<table>
<thead>
<tr>
<th>Variables</th>
<th>DCS</th>
<th>Prediction</th>
<th>Error%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam temperature</td>
<td>434</td>
<td>439</td>
<td>1.0</td>
</tr>
</tbody>
</table>

In Table 2 a comparison between measured and predicted data from the simulation for full load and partial load is presented.
Table 1: Thermophysical properties of the biomass.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value 1</th>
<th>Value 2</th>
<th>Value 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluegas temperature after cyclone (°C)</td>
<td>550</td>
<td>566</td>
<td>2.9</td>
</tr>
<tr>
<td>Fluegas temperature before cyclone (°C)</td>
<td>551</td>
<td>576</td>
<td>4.6</td>
</tr>
<tr>
<td>Steam temperature after cyclone (°C)</td>
<td>366</td>
<td>353</td>
<td>-3.6</td>
</tr>
</tbody>
</table>

As can be seen the absolute error varies between 0 and 5 %. If the purpose of the simulation model would be to have an as accurate model as possible, this might be problematic, but in this case we want to compare the model prediction with measured data many times in a time series to determine the trend.

Similar verifications have been performed for the anaerobic digester and a pilot black liquor gasification process. In Derbal et al. (2009), Donoso-Bravo et al. (2011) and Lübken et al. (2007) others anaerobic digestion models are described including verification of the models.

A dynamic simulation approach has been proposed. This approach has been used for the simulation of energy conversion processes for diagnostics and process control. The use of the advanced object oriented language Modelica has considerably reduced the modelling efforts thanks to the reusability of the system components and interchange ability between processes. The main feature of the proposed modelling and simulation approach is that the chemical composition of the fuel and other sub products can be followed through the whole process. As previously named the heterogeneity of the incoming raw material is the cause of multitude process upsets, making the proposed approach interesting.

The comparison of the simulation results with the real process results allows determining process upsets. The physical models can be combined with other type of models like here Bayesian nets or Multivariate models to obtain a decision support and prediction tools as in Widarsson and Dotzauer (2008).

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REFERENCES


Fig. 4. Biogas production 2006 compared to 2010.

In Fig. 4 the improvements in the biogas production from first quarter 2006 to last quarter 2010 are depicted. This was the result of several different actions including modeling of the process to get a better understanding of how to control the process in a better way.

4. CONCLUSIONS

In many occasions energy conversion processes are based on the same physical laws and can be therefore modelled in similar ways. The construction of a Modelica energy conversion library, allows reuse of the designed classes. This means that with not so much effort new energy conversion processes can be modelled. Fig. 1 shows the similarities and differences between three energy conversion processes that can be considered as completely different processes but with many synergies when modelling can be found.


