EMSO: Environment for Modeling, Simulation and Optimization of Biorefineries

Argimiro R. Secchi

Chemical Engineering Program – COPPE
Universidade Federal do Rio de Janeiro
Technological Center, Rio de Janeiro – RJ, Brazil

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Chemical Engineering Program
✓ Founded in 1963
✓ First department of COPPE, origin of the Institute
✓ First to offer Graduate Courses in Engineering in Brazil

2018
Chemical Engineering Program

Research Areas

✓ Kinetics and Catalysis
✓ Modeling, Simulation and Control of Chemical Processes
✓ Biotechnology and Environmental Processes
✓ Membrane Separation Processes
✓ Polymer Engineering
✓ Applied Thermodynamic
✓ Thermofluidynamics
✓ Interfacial Phenomena
Chemical Engineering Program

Solutions for Process Control and Optimization
COPPE/UFRJ
EMSO: Environment for Modeling, Simulation and Optimization of Biorefineries

• Motivation
• Environment for Modeling, Simulation and Optimization
• Biorefinery Modeling
• Biorefinery Simulation
• Biorefinery Optimization for 1G+2G Bioethanol Production
• Final Remarks
Motivation

- High dependence on fossil fuels
- Growing energy needs
- Increasing GHG emissions
- Opportunities for renewable resource

- Total Emissions in 2012 = 6,526
  Million Metric Tons of CO₂ equivalent


- Energy consumption by sector

- Energy demand increases 41% between 2012 and 2035

- Global ethanol production 2013 (million gallons)

- Global energy consumption by fuel (2011)

- Waste and wastewater, 3%
- Energy supply, 26%
- Forestry, 17%
- Agriculture, 14%
- Industry, 19%
- Residential & Commercial buildings, 8%
- Transport, 13%

- Source: IEA, 2013
- Source: BP, 2014
- Source: IPCC, 2007; EPA, 2012
- Source: USDA-FAZ, 2014

Motivation

Global production of biofuels

Industrial routes for conversion of biomass

Motivation

Many process synthesis and design alternatives

**SHF:** Separate Hydrolysis and fermentation. Low efficiency. Older technology.

**SSF:** Prevents enzyme inhibition by product. Disadvantages in operating conditions (≠ optimal cond.)

**SSCF:** Only one bioreactor.

**CBP:** Only one microorganism and one bioreactor.

Motivation

Several equipment types and operating modes

- Batch
- Fedbatch
- Continuous
- Continuous with product separation
- Continuous tubular
- Fluidized bed

... and many others!
Motivation

Opportunities for process optimization

Need Computer Aided Process Engineering (CAPE) Tools!

- Furlan et al. (2015), Computer Aided Chemical Engineering, 37, 1349-1354.
EMSO stands for “Environment for Modeling, Simulation, and Optimization”

Development started in 2001 (by Rafael P. Soares), written in C++ language

Available in Windows and Linux

Models are written in an object-oriented modeling language

Equation-oriented simulator and optimizer

Computationally efficient for dynamic and steady-state simulations

Continuous improvements through ALSOC project:

http://www.enq.ufrgs.br/alsoc
Thermodynamic and Physical Properties – Plugin

Data bank with about 2000 pure compounds

Thermodynamic models:
- Ideal Gas
- RK
- SRK
- PR
- APR
- ASRK
- CPA
- GERG2008
- Ideal Liquid
- Wilson
- NRTL
- UNIFAC
- UNIQUAC
- F-SAC

Mixture properties calculation
All equipments or modules are simultaneously evaluated (Block decomposition can be used to explore sequential solution).

Open-source Modeling

Equipment contain only chemistry and physics of the model

ex: EMSO, Ascend, Jacobian, gPROMS, AspenDynamics, EcosimPro
A process flowsheet model can be hierarchically decomposed:
Object-Oriented Modeling

- Abstract model
  - Mass balance
  - Energy balance
  - Thermodynamic equilibrium
  - Mol fraction normalization

- Concrete model (ideal tray)
  - Liquid flow model
  - Vapor flow model
  - Efficiency model

- Concrete model (real tray)
Examples of general-purpose object-oriented modeling languages:

- **ABACUSS / JACOBIAN** (Barton, 1999)
- **ASCEND** (Piela, 1989)
- **Dymola** (Elmqvist, 1978)
- **EcosimPro** (EA Int. & ESA, 1999)
- **EMSO** (Soares and Secchi, 2003)
- **gPROMS/Speedup** (Barton and Pantelides, 1994)
- **Modelica** (Modelica Association, 1996)
- **ModKit** (Bogusch et al., 2001)
- **MPROSIM** (Rao et al., 2004)
- **Omola** (Andersson, 1994)
- **ProMoT** (Tränkle et al., 1997)

- **Separation Systems**
  - Dynamic Flash
  - Steady-State Flash
  - Dynamic Condenser
  - Steady-State Condenser
  - Dynamic Reboiler
  - Steady-State Reboiler
  - Partial Reboiler
  - Equilibrium Stage - Tray
  - Splitter
  - Mixer
  - Cylindrical Tank
  - Horizontal Cylindrical
  - Column Section
  - Distillation Column with Dynamic Condenser and Reboiler
  - Distillation Column with Thermosyphon Reboiler and Sub-cooling
  - Distillation Column with Thermosyphon Reboiler and Dynamic Condenser
  - Distillation Column with Kettle Reboiler and Sub-cooling
  - Rectifier Column
  - Rectifier Column with Sub-cooling
  - Stripping Column with Reflux
  - Stripping Column with Sub-cooled Reflux
  - Absorption Column with Reflux
  - Absorption Column with Sub-cooled Reflux
  - Stripping Column with Kettle Reboiler
  - Stripping Column with Thermosyphon Reboiler
  - Absorption Column with Kettle Reboiler
  - Absorption Column with Thermosyphon Reboiler

- **Controllers**
  - PID Controllers (series, parallel, AW, AWBT)
  - Incremental PID Controllers (series, parallel, AW, AWBT)
  - Lead-Lag, Lag
  - Comparator, Sum, Ratio, Multiply, HiLoSelect
  - IAE
  - ISE

- **Heat Exchangers**
  - Simplified Shell-Tube Heat Exchanger
  - Rigorous Shell-Tube Heat Exchanger
  - Discretized Shell-Tube Heat Exchanger
  - Multi-Streams Heat Exchanger - MHeatex
  - Heat Exchanger - Heater and Cooler
  - Double Pipe Heat Exchanger
  - Plate Heat Exchanger

- **Reactors**
  - CSTR
  - PFR
  - Gibbs
  - Equilibrium
  - Batch
  - Fed Batch

- **Pressure Changers**
  - Pumps
  - Turbines
  - Compressors
  - Valves

- **Didactic Models**
  - Fogler’s book Exercises
What can I do with EMSO?

- Dynamic and steady-state simulation
- Steady-state optimization (NLP, MINLP)
- Dynamic and steady-state parameter estimation
- Steady-state data reconciliation
- Process monitoring and inferences with OPC communication
- Build bifurcation diagram (interface with AUTO for DAEs)
- Sensitivity analysis and case study (surface response)
- Linearization of nonlinear dynamic system
- State estimation and model updating (EMSO-CEKF)
- Dynamic simulation with SIMULINK/SCICOS (interface with MATLAB/SCILAB)
- Add new solvers (DAE, NLA, NLP)
- Add external routines using the Plugins resource
Biorefinery Modeling

EMSO as platform for Sugarcane Virtual Biorefinery (since 2012)
## Biorefinery Modeling

### Physico-chemical properties

<table>
<thead>
<tr>
<th>#</th>
<th>Component</th>
<th>#</th>
<th>Component</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>water</td>
<td>17</td>
<td>HMF (hydroxymethylfurfural)</td>
</tr>
<tr>
<td>2</td>
<td>sucrose</td>
<td>18</td>
<td>glycerol</td>
</tr>
<tr>
<td>3</td>
<td>glucose</td>
<td>19</td>
<td>unknown sugars</td>
</tr>
<tr>
<td>4</td>
<td>xylose</td>
<td>20</td>
<td>MEG (ethylene glycol)</td>
</tr>
<tr>
<td>5</td>
<td>ethanol</td>
<td>21</td>
<td>sulfuric acid</td>
</tr>
<tr>
<td>6</td>
<td>CO$_2$</td>
<td>22</td>
<td>phosphoric acid</td>
</tr>
<tr>
<td>7</td>
<td>CO</td>
<td>23</td>
<td>impurities</td>
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<tr>
<td>9</td>
<td>oxygen</td>
<td>24</td>
<td>cellobiose</td>
</tr>
<tr>
<td>9</td>
<td>nitrogen</td>
<td>25</td>
<td>ammonium hydroxide</td>
</tr>
<tr>
<td>10</td>
<td>hydrogen</td>
<td>26</td>
<td>cellulose</td>
</tr>
<tr>
<td>11</td>
<td>methane</td>
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<td>hemicellulose</td>
</tr>
<tr>
<td>12</td>
<td>ammonia</td>
<td>28</td>
<td>ash</td>
</tr>
<tr>
<td>13</td>
<td>lignin</td>
<td>29</td>
<td>enzyme</td>
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<tr>
<td>14</td>
<td>xylan</td>
<td>30</td>
<td>yeast</td>
</tr>
<tr>
<td>15</td>
<td>acetic acid</td>
<td>31</td>
<td>calcium hydroxide</td>
</tr>
<tr>
<td>16</td>
<td>furfural</td>
<td>32</td>
<td>calcium phosphate</td>
</tr>
</tbody>
</table>

Many chemical species not present in petrochemical-oriented database
Biorefinery Model Library

Biomodel

1. assumptions
2. energy stream
3. main stream
4. water stream

Accessories
1. duplicator and selector
2. tank
3. valve

Heat exchangers
1. heater
2. water heater
3. heat exchanger
4. hybrid heat exchanger
5. water heat exchanger

Mixers and splitters
1. mixer and splitter
2. water mixer and splitter
3. hybrid mixer
4. splitter heat
5. splitter power

Pressure changers
1. compressor
2. isenthalpic valve
3. pump
4. water pump
5. turbine
6. steam turbine

Reactors
1. boiler
2. digester
3. enz. hydrolysis
4. fermenter
5. liming tank
6. phosphate tank
7. pre-treatment
8. stoic. reactor

Separators
1. centrifuge
2. cleaning
3. column
4. decanter
5. dry cleaning
6. evaporator
7. filter
8. flash
9. water flash
10. mill
11. separator
12. sieve
13. absorption tower

Flowsheets
1. Examples of flowsheets
Biorefinery Modeling

Block Diagrams
Biorefinery Simulation

1G + 2G ethanol-from-sugarcane production plant

Biorefinery Simulation

Co-generation plant using biomass or lignin
Biorefinery Optimization

Biorefinery Optimization

Retro-Techno Economic Analysis

iso-economics NPV = 0

iso-economics NPV = 0

\[
\text{Reaction yield} \quad \text{Biocatalyst yield}
\]

[Graph showing reaction yield and biocatalyst yield against solid mass fraction in the hydrolysis reactor]

Final Remarks

- CAPE tools are available for bioprocess synthesis and design;
- Simulation and optimization of biorefineries illustrate the potential of the developed model library;
- Physico-chemical properties database need to be enlarged;
- The power and availability of computer hardware and software have increased our ability to model complex phenomena in biochemical processes. In fact, we are probably limited now more by what can or cannot be measured experimentally, than by techniques for solving equations;
- Particular importance are model-based state estimation techniques which compensate for the scarcity of online sensors for bioprocesses.
Professors
Antônio J.G. Cruz (UFSCar)
Argimiro R. Secchi
Caliane B.B. Costa (UEM)
Elba P.S. Bon (Bioetanol)
Felipe F. Furlan (UFSCar)
Frederico W. Tavares
Kese P.F. Alberton, EQ
Roberto C. Giordano (UFSCar)
Maurício B. de Souza Jr.
Príamo A. Melo Jr.
Tito L.A. Moitinho

Engineers:
Bruno L. Nogueira
Dasciana Rodrigues (Embrapa)
Jurgen L. Bregado
Ricardo S. Teixeira (Bioetanol)
Rodrigo R.O. Barros (Bioetanol)
Rossano Gambetta (Embrapa)

PhD students:
Alex F. Teixeira
Ataíde S. Andrade
Caio F. C. Marcellos
Daniel M. Thomaz
Eliza H. C. Ito
Felipe C. Cunha
Javier A. Angarita
Jeiveison G. S. S. Maia
Leonardo D. Ribeiro
Maria Rosa T. Goes
Rafael B. Demuner
Reinaldo C. Spelano
Roymel R. Carpio
Sergio A. C. Giraldo
Thamires A. L. Guedes

Post-Docs:
José Mauel G. T. Perez
Leonardo S. Souza
Simone C. Miyoshi

MSc students:
Allyne M. dos Santos
André F. F. Souza
María Jimena F. Quagliata
Mariana Carvalho
Mariana K. Moro
Mario G. Neves Nt.
Otávio F. Ivo
Pedro C. N. Ferreira
Thiago C. d’Ávila
Vitor P. Paixão

Undergrad. students:
Bruno Bez
Carlos M. M. Fonseca
Isabella Q. Souza
Lucas F. Bernardino
Lucas Marques
Pedro Delou
Silvio Cisneiros Nt.
Thales S. M. Gama
Víctor C. Gomes

Secretariat: Rosemary Cezar
You are very welcome to visit us
... thank you for your attention!

Process Modeling, Simulation and Control Lab
- Prof. Argimiro R. Secchi, D.Sc.
- Phone: +55-21-3938-8307
- E-mail: arge@peq.coppe.ufrj.br

Prof. Maurício B. de Souza Jr., D.Sc.
- Phone: + 55-21-3938-7315
- E-mail: mbsj@eq.ufrj.br


http://www.enq.ufrgs.br/alsoc


References


