COMPUTER SIMULATION OF SULPHURIC ACID PLANTS

By:
Guy Cooper, P. Eng
Kim Nikolajsen, PhD
Brian Ferris, P. Eng

Of:
NORAM Engineering and Constructors Ltd.
Vancouver, BC

For:
Lead Zinc Sulfuric Acid Short Course
October 3, 2010,
Vancouver, BC
Agenda

- Why Simulate Your Plant
- Challenges
- History
- Tools Available
- Modeling an Acid Plant (steady-state)
- Dynamic Modeling
- Summary
Who is NORAM?

- Based in Vancouver
- Founded in 1988
- 100 employees – chemical and mechanical
- Performed over 144 acid plant studies
- Supplied over 150 acid plant components
- Own a fabrication shop, 80 employees
- Licensor to Simon Carves UK - 450 mtpd acid plant UAE
- Licensor to Bateman South Africa – Two 2850 mtpd acid plants Madagascar
NORAM’s Sulfuric Acid Equipment

NORAM offers state-of-the-art designs and technologies to the Sulfuric Acid Industry. NORAM equipment improves your plant’s performance by providing lower pressure drop, increased capacity, reduced operating costs and a longer life.

Suite 1800 - 200 Granville Street, Vancouver, British Columbia V6C 1S4 Canada
tel: 604 681 2030  fax: 604 683 9164  email: acid@noram-eng.com
www.noram-eng.com
Axton Fabrication Shop
2010 Winter Olympics - Vancouver
Why Simulate Your Acid Plant?

- Allows you to change process inputs and see how your plant will perform
- Identify process bottlenecks
- Determine benefits of new equipment
- Confirm accuracy of process measurements
- Improve plant control; parametric analysis

In general, allows a better understand of your acid plant

Sounds great, but… it ain’t easy to model and get the above benefits!
Generic Sulphuric Acid Plant
Sulphur Burning

Gas Process Flow Diagram
Challenges in Simulating Your Acid Plant

- Don’t trust all your process readings (some are flakier than others)
- Missing important equipment information
- Don’t know what software to use
- Software may not be easy to use
- Don’t have time
History of Process Simulators

• In-House Process Simulators
  • Popular 1960’s-1980’s
  • Created by in-house engineers of major oil & gas, chemical companies
  • Ran on computer mainframes

• Simulation Sciences, *Process*, later, *PRO/II*
  • *Process* Ran on Main Frame
  • Appeared on the scene late ’70’s
  • PRO/II came out about 1990. PC-based batch operation

• Hyprotech, *Hysim*, later *Hysys*
  • First major PC Based Simulation
  • Calgary Based, U of C, appeared in mid ’80’s
  • Interactive, backward calculation capability gave increased flexibility
  • Hysys introduced in the ’90’s was Windows version of Hysim
  • NORAM used it for gas side. Acid side done on spreadsheet
History of Process Simulators (cont’d)

- Aspen Technology Inc. *Aspen Plus, & Hysys*,
  - Created in 1981. Joint research project MIT and US DOE. Advanced System for Process Engineering (ASPEN)
  - Acquired Hyprotech in 2004 and divested Hysys code to Honeywell (FTC)
  - Offer suite packages

- Honeywell, *UniSim*, formerly *Hysys*
  - Bought the code to Hysys in 2004
  - Markets under the name UniSim
  - Offer suite packages

The suite packages offered include steady state, dynamic modeling, special physical property packages, heat exchangers, pipe pressure drop, plant optimization, basic engineering, … next presentations for sulphuric acid plant courses
Tools Available
(for Process Simulation)

• Commercial Generic Simulators
  • Aspen Hysys, Apen Plus, Honeywell Unisim
  • Need to develop equipment models and select property packages
  • Somewhat flexible for new equipment
  • Lease costs can be high

• Third Party Dedicated Software
  • Shiv Shukla, India Sulphuric, and others
  • Limited in flexibility
  • Pre-configured
  • Relatively low cost <$2000
Tools Available (cont’d)
(for Process Simulation)

• **User Created Spreadsheet Models**
  • User creates models of individual equipment or entire acid plant
  • Requires good understanding of unit operations
  • Requires source of physical property data correlations
  • Provides good flexibility in data input/output
  • Requires checking of connectivity
  • Requires good documentation and internal notes for use by others
Tools Available (cont’d)
Suite Packages

Economic Evaluation Products

- Aspen Process Economic Analyzer (APEA)
- Aspen Capital Cost Estimator (ACCE)
- Aspen In-Plant Cost Estimator (AICE)
Tools Available (cont’d)

Suite Packages

Compare based on Technology & Economics!

**Option 1**
- Aspen Plus Simulation
- HYSYS Simulation
- Economic Analysis

Capital = $30M; Operating = $13M/yr

**Option 2**
- Aspen Plus Simulation
- HYSYS Simulation
- Economic Analysis

Capital = $28M; Operating = $11M/yr
Aspen HYSYS Benefits

Aspen HYSYS is a proven, industry-standard solution with over twenty years of use in the field. Customers have recognized and reported:

- $15 million per year in incremental profitability from process optimization
- $10 million per year in capital savings resulting from improved designs
- $1 million per year of reduced engineering cost

Aspen Plus is a proven, industry-standard solution with over twenty years of use in the field. Customers have recognized and reported:

- $15 million per year in incremental profitability from process optimization
- $10 million per year in capital savings resulting from improved designs
- $1 million per year of reduced labor costs from improved conceptual engineering workflow
Physical Property Prediction

• Important part of simulation is ensuring accurate physical property prediction
• In simple terms, Equations of State are formula and coefficients used to predict component and stream physical properties under varying conditions
• For sulphuric acid plants, gas, steam and acid generally use separate equations of state to predict Cp, Volume, Density, conductivity, and so forth

Various Equations of State

1. Overview
2 Historical
   2.1 Boyle’s law (1662)
   2.2 Charles’s law or Law of Charles and Gay-Lussac (1787)
   2.3 Dalton’s law of partial pressures (1801)
   2.4 The ideal gas law (1834)
   2.5 Van der Waals equation of state
3 Major equations of state
   3.1 Classical ideal gas law
4 Cubic equations of state
   4.1 Van der Waals equation of state
   4.2 Redlich–Kwong equation of state
   4.3 Soave modification of Redlich-Kwong
   4.4 Peng-Robinson equation of state
   4.5 Elliott, Suresh, Donohue equation of state
5 Non-cubic equations of state
   5.1 Dieterici equation of state
6 Virial equations of state
   6.1 Virial equation of state
   6.2 The BWR equation of state
7 Multiparameter equations of state
   7.1 Helmholtz Function form
8 Other equations of state of interest
   8.1 Stiffened equation of state
   8.2 Ultrarelativistic equation of state
   8.3 Ideal Bose equation of state
9 Equations of state for solids

Physical Property Prediction

• Important part of simulation is ensuring accurate physical property prediction
• In simple terms, Equations of State are formula and coefficients used to predict component and stream physical properties under varying conditions
• For sulphuric acid plants, gas, steam and acid generally use separate equations of state to predict Cp, Volume, Density, conductivity, and so forth
Physical Property Prediction (cont’d)

Summary

- The SO$_2$·H$_2$O·H$_2$SO$_4$ system in the HyS cycle poses significant modeling challenges
- Existing models for SO$_2$ solubility in sulfuric acid are deficient
  - Speciation most likely not correct
  - Differences between models lead to different performance predictions for SO$_2$-handling operations
- Aspen Plus™ modified Oleum model needs three distinct parameter/speciation sets to describe SO$_2$·H$_2$O·H$_2$SO$_4$ system
  - divided into low-/high-temperature and SO$_2$ VLE/VLLE regions
  - Good performance within each regime, but discontinuous transitions
- OLI Systems’ Mixed Solvent Electrolyte model gives comparable fit
  - No need to change model for temperature, VLLE reasons
  - Can be used as a property option set within Aspen Plus™
Modeling an Acid Plant

Unit Operations

• Sulphur Furnace – Gibbs or Conversion model reactor
• Acid Towers – Component splitter, absorption module
• Blower – Compressor module
• Heat Exchanger/Acid Cooler – Heat exchanger module
  • UA input and predict two temperatures, or,
  • Three of four temperatures are input and fourth predicted
• Converter – Reactor module
  • Conversion. Input conversion.
  • Equilibrium. Input approach to equilibrium
Modeling an Acid Plant

Building a model of the plant

• Get out plant process flow diagrams and piping and instrument diagrams
• Get exchanger drawings or rating sheets
• Take pressure profile and gas flow for starting point of model
• Record temperatures and flows of plant streams
• Enter stream and equipment data
• Model plant

It’s that easy. But most likely not!
Modeling an Acid Plant

Modeling blower performance from blower curve
Modeling an Acid Plant

Custom-built Spreadsheet

- Spreadsheet Set-Up
  - Mass and energy balances are simulated for the equipment components
  - Gas: \( C_p \) vs. Temperature for each component is from validated references
  - Acid: Solution enthalpy vs. Concentration and Temperature
  - Water: \( C_p \) is from steam tables

\[
H = \int_{T_{REF}}^{T} \sum_i (y_i C_{pi}) dT
\]

- Columns in spreadsheet are for streams
- Unit operations carried out on the components in the streams
- For SO2 to SO3 reaction enter approach to equilibrium or conversion
### User Created Spreadsheet Models

#### Extract of Spreadsheet Model of Sulphuric Acid Plant

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
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<td>Viscosity</td>
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</table>
Modeling an Acid Plant (cont’d)

- User Created Spreadsheet Models
### User Created Spreadsheet Models

#### Modeling an Acid Plant (cont’d)

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
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<th>G</th>
<th>H</th>
<th>I</th>
<th>J</th>
<th>K</th>
<th>L</th>
<th>M</th>
<th>N</th>
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<tbody>
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<td>1</td>
<td>HP pre-rating</td>
<td>Basis</td>
<td>Current</td>
<td>Design</td>
<td>Bypass pressure balance</td>
<td>Main flow through HP tubes</td>
<td>[ \text{At} \Delta P \text{ (g)} ]</td>
<td>91X</td>
<td></td>
<td></td>
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<tr>
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<tr>
<td>3</td>
<td>SO2 conc %</td>
<td>( % )</td>
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<td>10.63%</td>
<td>10.25%</td>
<td>( % )</td>
<td>10.51%</td>
<td>10.63%</td>
<td>10.25%</td>
<td>( % )</td>
<td>10.51%</td>
<td>10.63%</td>
<td>10.25%</td>
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<td>Vol. Head</td>
<td>0.01 m</td>
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![Diagram](image-url)

**Fig. 14.19.** Loss coeffcients vs. Val

**Fig. 14.21.** Driving flow branch and loss coefficient $K_{L}$. 

- **Figures and Tables**: Referencing key figures and tables pertinent to the modeling of an acid plant, focusing on pressure drop, heat transfer, and effective factors, with a special emphasis on the impact of HP pre-rating and production rate on system efficiency.

- **Tables and Calculations**: Highlighting critical dimensions, pressures, and efficiency metrics, ensuring all calculations align with industry standards and best practices.

- **Integration of Key Parameters**: Incorporating essential parameters such as SO2 concentration, flow rates, and effective LMTD to provide a comprehensive overview of performance metrics.

- **Graphs and Diagrams**: Utilizing graphs and diagrams to visually represent the relationship between variables, such as loss coefficients and various flow rates, enhancing understanding and application in real-world scenarios.

- **Model Validation**: Discussing methods for validating the model against real-world data, ensuring accuracy and reliability in the simulation.

- **User Interface**: Describing the user interface for the spreadsheet model, including key elements for easy navigation and data entry.

- **Applications**: Exploring potential applications of the model in the design and optimization of acid plants, emphasizing its versatility across different industrial settings.

- **Future Enhancements**: Suggesting areas for future enhancements, such as integration with real-time data feeds and advanced predictive analytics, to improve model performance and reliability.

- **Conclusion**: Concluding with a summary of the key findings and implications, reiterating the significance of the model in advancing the field of acid plant design and operation.

- **References**: Citing relevant literature and sources used in the development of the model, supporting the methodology and data presented.

- **Appendices**: Including supplemental materials such as additional equations, calculations, and detailed descriptions of model components, providing a comprehensive resource for further study.

- **Outlook**: Discussing potential future developments and advancements in the field of acid plant modeling, envisioning the role of such models in shaping the future of industrial process design and optimization.
Modeling an Acid Plant (cont’d)

- User Created Spreadsheet Models

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Custom-built Process Simulation
Commercial Simulation Process Flow Diagram

Diagram showing the process flow for sulfuric acid plants, including sulfur burning, heat exchanges, converters, absorbers, dryers, pumps, and product collection.
Dynamic Modeling an Acid Plant

- Useful when conditions fluctuate
- Can help setup process controls
- Requires all the information for steady state simulation plus
  - Thermal mass
  - Residence time
  - Valve description
- Use commercial package or create your own
Custom Built Dynamic Process Simulation
Commercial Program for Dynamic Simulation

Figure 2a. Aspen HYSYS Controlled from DMCplus GUI

Figure 2b. Aspen HYSYS Acting like the Real Plant
Commercial Program for Dynamic Simulation

Aspen DMCplus Controller

Step-Test Results

Controlled Variables

FeedForwards

Manipulated Variables
Summary

• Process simulation tools can be useful
• Require work for meaningful results
• Plants have several options for simulation
• May require consultant for assistance (unbiased promotion!)
Thank You
and Good Day