Agenda

• Current practices in design of batch scheduling
• Improvements made possible with
  – Rigorous modeling methodology
  – Microsoft Excel™ to drive a schedule in a simulator
• Example using CITRON (new process)
• Example using WINTEK (existing optimization)
• Summary & suggested procedure
Current practices in design of batch scheduling

• Methods
  – Best guess & experience
  – Lab scale & pilot scale testing
  – Use a basic simulation

• Pros
  – Fast
  – Fairly easy
  – Gives a basic time and heat duty analysis

• Cons
  – Suboptimal schedule times
  – Might not account for equipment/process limitations
  – Difficult to do safety analysis until after process is running
CITRON (current practice)

Recover 120 kgs of 99.9999% pure Citronellal from 170 kgs essential oil using a 500L pot still with a 10ft packed column.
CITRON (current practice)

Accumulator Contents vs. Time

Bottoms Contents vs. Time
What have we learned from the model?

• Heat duty/flow/time relationship
• Basic operation steps/timing
• Limited equipment sizes and specifications:
  – Heating requirements
  – Condenser requirements
  – Column dimensions
CITRON Dynamic (advanced practice)

• Expand our previous example to include
  – Rigorous heat exchanger geometry and performance
  – Event sequencing using DATAMAP to Microsoft Excel
  – Utilities modeling
  – Column metal heat transfer
  – Heat duty / cooling water on control
  – Dry column startup to total reflux
  – Detailed engineering, e.g., nitrogen sweep on vessel, insulation, etc.
A schedule of events is made in Excel and must be connected to CHEMCDAD:

<table>
<thead>
<tr>
<th>Schedule of Events</th>
<th>CW Valve mode</th>
<th>CW Valve Opening</th>
<th>Total reflux</th>
<th>Product Tank</th>
<th>Waste Tank</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time(min)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>36</td>
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<tr>
<td>21</td>
<td>4</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Schedule of heat duty to pot

- 0 Startup
- 0 Lower heat duty
- 0 Open CW Valve
- 0 Switch off Total reflux
- Heater off, drain to tank
- CW off
CHEMCAD to Excel connection

CHEMCAD sends time information to Excel cell A2 via datamap

Excel uses time, schedule, and VLOOKUP() function to determine values of process variables

CHEMCAD collects the current time step data from row 2 of the Excel sheet and enters it into the flowsheet via datamap

Time step sent from CHEMCAD

Duty sent back to CHEMCAD for the current time step
Accumulator Contents vs. Time

- CITRONELLAL
- CITRONELLOL
- GERANIOL

Bottom Contents vs. Time

- Initial vapor boiling
- Column holdup is filled
- Column taken off total reflux
- Heat turned off, outlet pump on

Mass (kg) vs. Time (minutes)
Comparison of CC-BATCH and CC-Dynamics

Column Bottom Flow

CC-DYNAMICS Simulation
CITRON Dynamic

- End of total reflux
- Reflux change gets to the bottom of column
- Onset of boiling, heating the column
- End of operation step, Column draining back to pot

CC-BATCH Simulation
CITRON

- End of total reflux, recall that CC-Batch starts t=0 at end of total reflux
- End of operation step
We learned from using dynamics:
• Detailed startup procedure
• Detailed operation steps/Sequence details
• Equipment performance limitations
• Vacuum load
• Utility demands
• Equipment optimization is now possible: checking condenser capacity, vacuum system capacity, column flood %, column insulation requirements, etc.
• Higher fidelity simulation provides higher fidelity economic calculation (campaign time and costs)
Skid mounted solvent dehydration plant

Stripping water from a solvent stream in a two bed adsorber (mol sieve) system. One bed is active and one bed is regenerating under vacuum. Process was already built and operational before modeling analysis.

Process is scheduled with a defined sequence for opening and closing valves to allow one bed to regenerate while the other adsorbs. Rigorous equipment and piping models and pressure/flow calculation included (allows for reversible flow).

Rigorous simulation allows us to simulate effect of malfunction (RB3 blowdown valve malfunction)
WINTEK Process Flowsheet

2 Adsorption beds
2 PID controls
10 Actuated ball valves
### WINTEK Datamap and Schedule

<table>
<thead>
<tr>
<th>Time step sent from CHEMCAD</th>
<th>Schedule of time events</th>
</tr>
</thead>
<tbody>
<tr>
<td>VLOOKUP Function to get P1 signal at current time step</td>
<td>Schedule of P1 actuation signal at different times</td>
</tr>
</tbody>
</table>

**Excel Workbook Path:** A_BREA_SIEVE_DLL_201.xls

**Excel Worksheet Name:** Sheet1

<table>
<thead>
<tr>
<th>Map Rule</th>
<th>CC Obj Type</th>
<th>CC Obj ID</th>
<th>Par ID</th>
<th>Component</th>
<th>WrkSht/Cell/Comment</th>
<th>Weight</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
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<td>To Worksheet</td>
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<td>Dynamic Time</td>
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<td>A2</td>
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<td>Dynamic time(Min)</td>
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<td>D2</td>
<td>1.00000</td>
<td></td>
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<tr>
<td>To CC Only</td>
<td>UnitOp</td>
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<td>Controller out...</td>
<td>&lt;None&gt;</td>
<td>E2</td>
<td>1.00000</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time step</th>
<th>sent from CHEMCAD</th>
</tr>
</thead>
<tbody>
<tr>
<td>BV1</td>
<td>P1</td>
</tr>
<tr>
<td>BV1</td>
<td>P1</td>
</tr>
<tr>
<td>BV1</td>
<td>P1</td>
</tr>
<tr>
<td>BV1</td>
<td>P1</td>
</tr>
</tbody>
</table>

**DV2**

- =VLOOKUP($A$2,$C$7:$P$27,2,TRUE)
RB3 is simulated blocked, preventing Bed 1 from blowing down properly. Effect is rigorously calculated.
WINTEK Adsorber Beds

Pressure Profiles of Adsorber Beds

- **Bed 1 outlet opens, absorbing**
- **Bed 2 outlet opens, absorbing**
- **Bed 1 blowdown is not opening, notice the pressure here**
- **Bed 2 blowdown opens**
- **Bed 1 blowdown is not opening, notice the pressure here**

**Legend:**
- Blue: Pressure of bed 1
- Orange: Pressure of bed 2
- Dotted: Sequence event
WINTEK Anhydrous Solvent Flowrate

Anhydrous Solvent Flow Rate

Bed 1 adsorbing
Bed 2 adsorbing
Bed 1 adsorbing
Bed 2 adsorbing
Bed 1 blowdown
Bed 2 blowdown
Bed 1 blowdown valve is disabled
Bed 2 blowdown
Bed 1 blowdown valve is disabled

Flow rate vs. Time
WINTEK Process Flowsheet: reversing flow

P3 and P4 open, flow is forward through one valve, reverse through the other.
WINTEK Sequence of outlet and regeneration flows out of adsorber beds
By using an optimization engine (either the built-in engine in CHEMCAD, or an external one connected to the Excel spreadsheet) the schedule of valve events can be optimized to maximize on-stream performance (blue area of chart).
What did we learn from our model?
• Discrete event scheduler with pressure and flow calculations (including reversible flow) allowed optimization of the process schedule
• Ability to identify and quantify
  – Bottlenecks
  – Sequence timing issues
  – Equipment limitations
  – Malfunction effects (bed 1 blowdown valve sticking)
  – Control loop tuning issues
• Ability to use the model for process scaling: process can be scaled up or down to meet customer requirements using the model before building/assembly
• Ability to optimize schedule of events
Suggested Procedure

1. Start with a simplified model (like CC-BATCH) to get heat duties, initial equipment sizes/specifications, and an initial timing/schedule

2. Build a rigorous dynamic model with as much detail as required (but no more than required) to solve the engineering problem (e.g., only add reversible flow if it is a concern)

3. Build an event sequence control scheme using DATAMAP and Excel starting with the information gathered in Step 1 above. Progressively improve the sequence by running the dynamic model with the scheduler
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