

# Unsteady-State Simulation Using CHEMCAD Steady-State

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# Agenda

- Challenges
- Presentation of 3 cases
- Limitations of this approach

# Challenges

- How Do We Handle the Concept of Time
- Representing Volume Using a Rate
- Dependence on Visual Basic (Unsteady State Modeling)

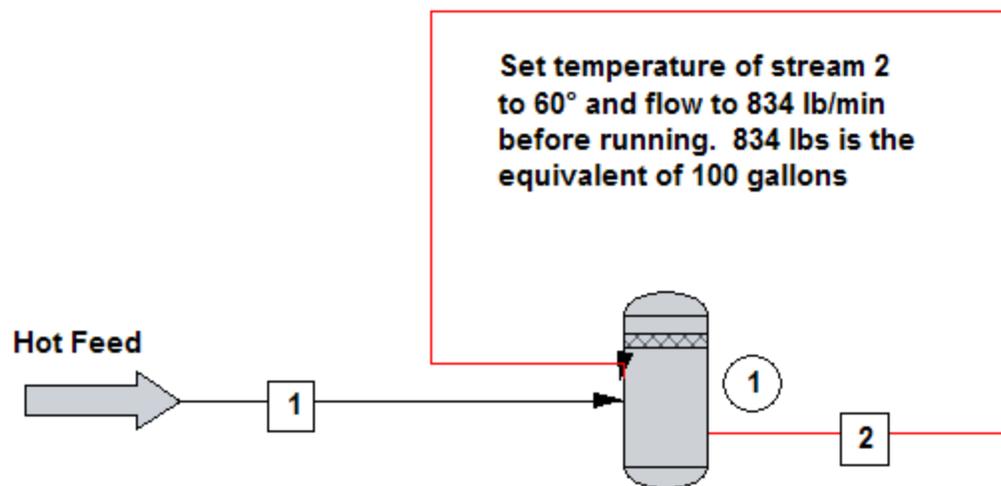
# 3 Example Cases

- Hot Water Tank (simple case)
- Acid – Base Neutralization
- Evaporation Simulation

# Simple Case - Defined

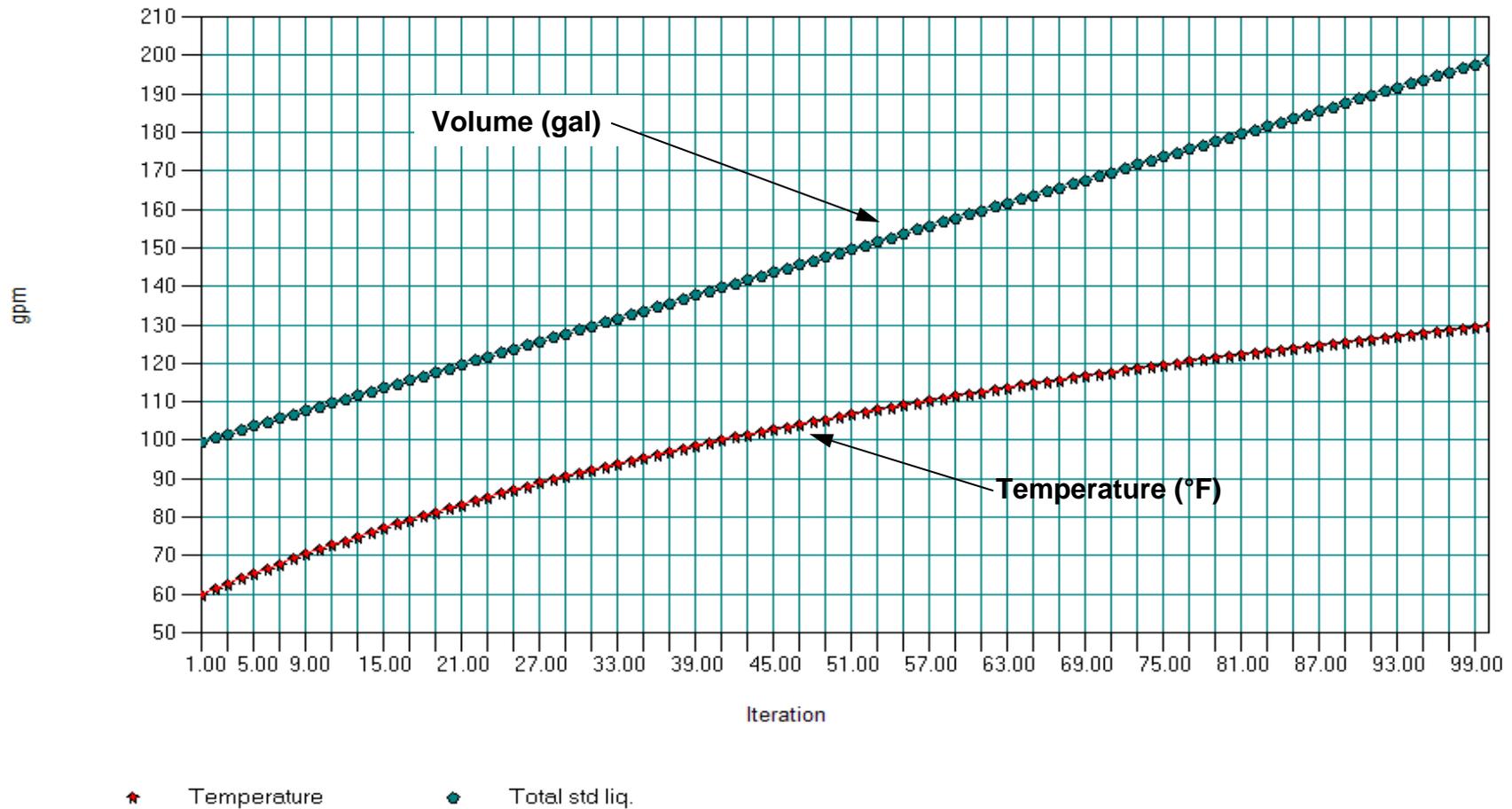
- Simulation models the addition of 1 gpm of a water stream at 200°F to a vessel which initially contains 100 gallons of water at 60°F
- Use of a recycle line with no side draw should result in increased volume in the Tank represented by stream 2 as time passes.
- The temperature in the “Tank” (Stream 2) should rise as the hot water is added

# Simple Case



# Simple Case - Results

Stream 2 Dynamic Plot



# Simple Case – Results, cont

- Tank Volume (stream 2) doubles after adding 1 gpm of water to an initial volume of 100 gallons over the course of 100 minutes.
- Tank temperature rises from 60°F to 130°F

# Key Points

- The number of iterations becomes a time scale, in effect tracking the time of the batch. The engineering unit selected for time is “minutes”. Therefore 100 iterations becomes 100 minutes elapsed.
- The time scale is very important and must be chosen carefully when designing the simulation.

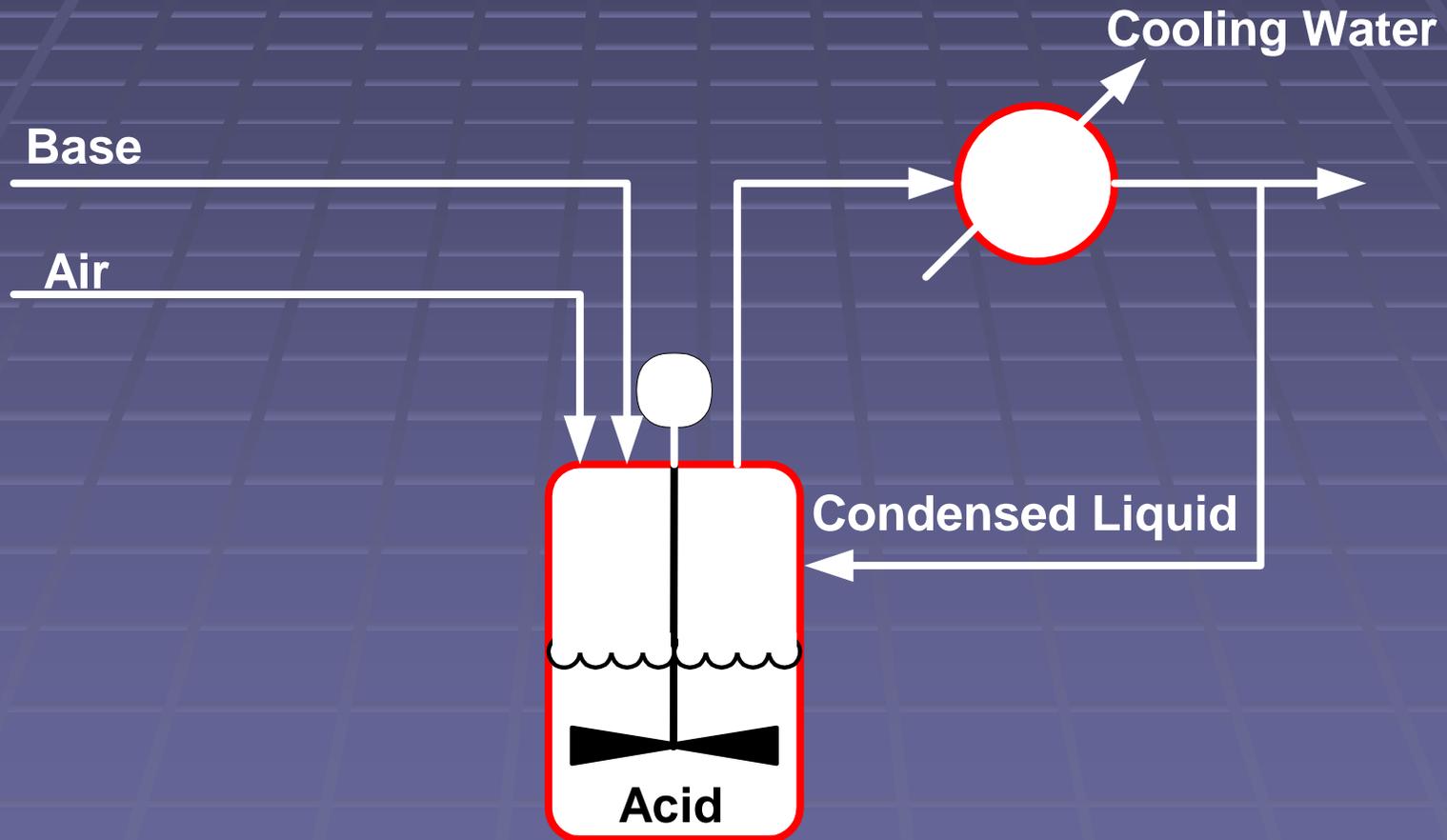
# Key Points, cont.

- Even though Stream 2 is actually a rate, it is also a volume. The rate becomes a cumulative volume because no side draw is present. Here is where the unsteady state behavior of the system is modeled.
- The time scale chosen for the model has no effect on the system volume. It does not matter whether the time scale is seconds, minutes or days; HOWEVER, the initial volume of Stream 2 MUST be the same: 100 gallons per second, 100 gallons per minute, 100 gallons per day. Each is equivalent to starting the simulation with 100 gallons of water in the tank.

# Acid Base Neutralization

- Client requested model of acid-base neutralization in a reactor with an air sweep
- A known volume of acid is charged to a reactor and a caustic stream is metered in over a period of time
- A condenser removes any acid in the ventilation stream

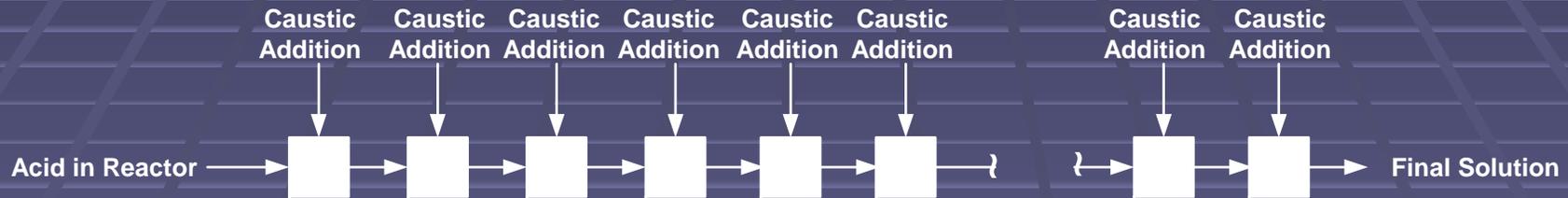
# Neutralization Schematic



# First Approach

- Use of a Mixer unit op in CHEMCAD to add all the base to all the acid in one iteration.
- Absolutely no representation of reality.

# Second Approach



- Blocks represent the entire system, i.e., all the unit ops daisy chained together
- Each block represents one time interval

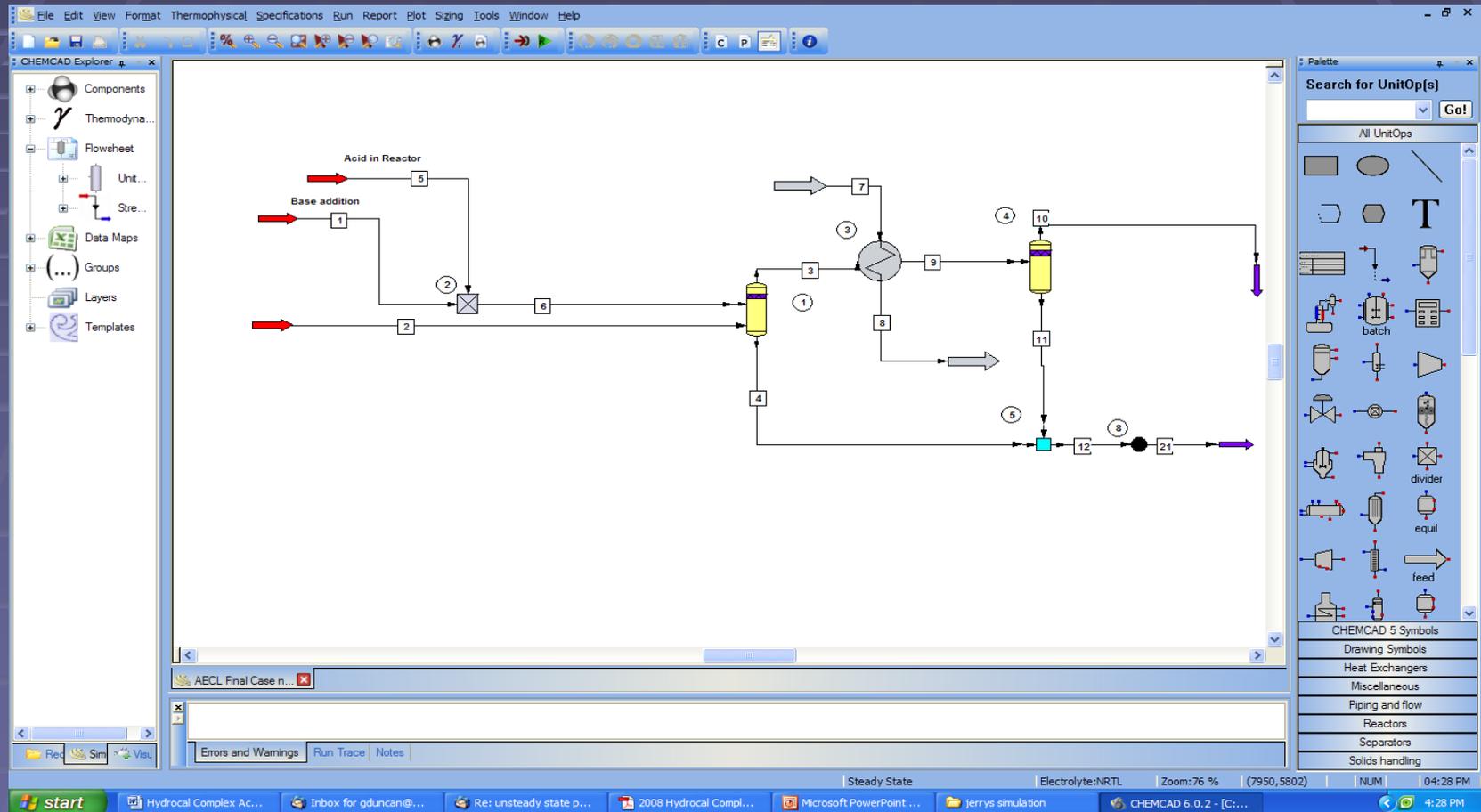
# Results of Second Approach

- Advantage:
  - More representative of actual system
- Disadvantages
  - Rigid time interval; changes to time means addition or removal of blocks
  - Complicated incorporation of unit ops and process streams (lots of mixing blocks)

# Third Approach

- Use of a stream reference to carry the reactor “volume” back to starting point
- Before running the simulation, stream 5 represents the total amount of acid initially charged to the reactor.
- When the simulation is run, the caustic is added to the reactor in mixing block 2.
- After each unit operation is complete in the iteration, stream 12 represents the initial acid content of the reactor, all previous caustic additions, and the additional amount of caustic fed to the reactor in the current iteration.
- A stream reference is used to transport the reactor volume back to stream 5 so that the next addition of caustic to the cumulative reactor from stream 1 can be made.
- Use of visual basic to control the batch time (actually controlling number of times the system undergoes one iteration)
- Demonstration

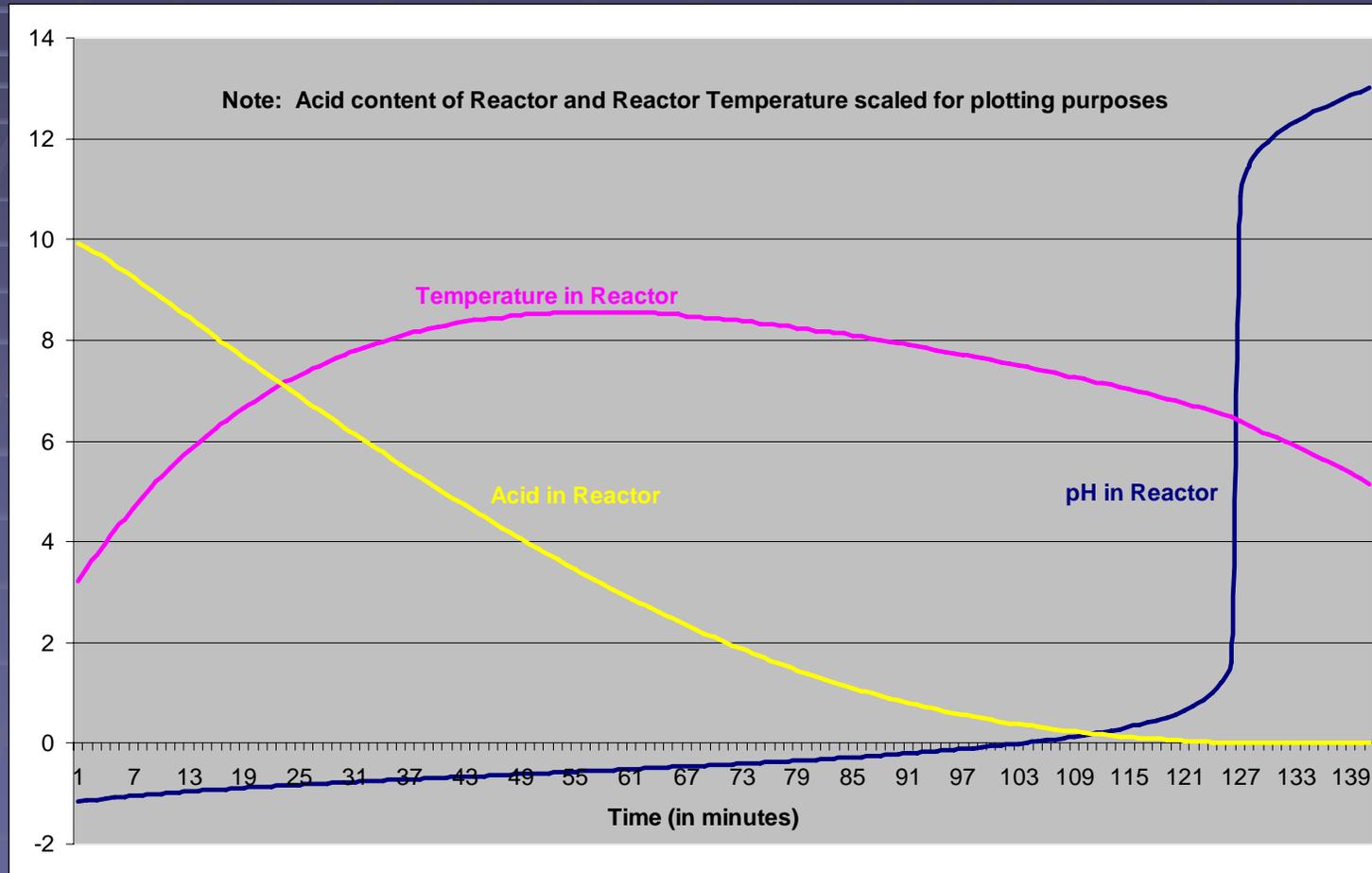
# Acid – Base Neutralization



# Results of Third Approach

- Amount of acid in the reactor is depleted over time
- pH of the batch demonstrates the typical equivalence point (quick transition from acidic solution to basic solution) encountered in titration of strong acids with strong bases
- Temperature rises due to heat of reaction, peaks, then slowly diminishes as the acid is depleted and is replaced with “cool” (lower than batch temperature) caustic

# Reactor Trends



# Results of Third Approach, cont.

- Accurate simulation of system as measured by comparison to data supplied by client
- Client has simulation that is relatively easy to manipulate for future modeling work

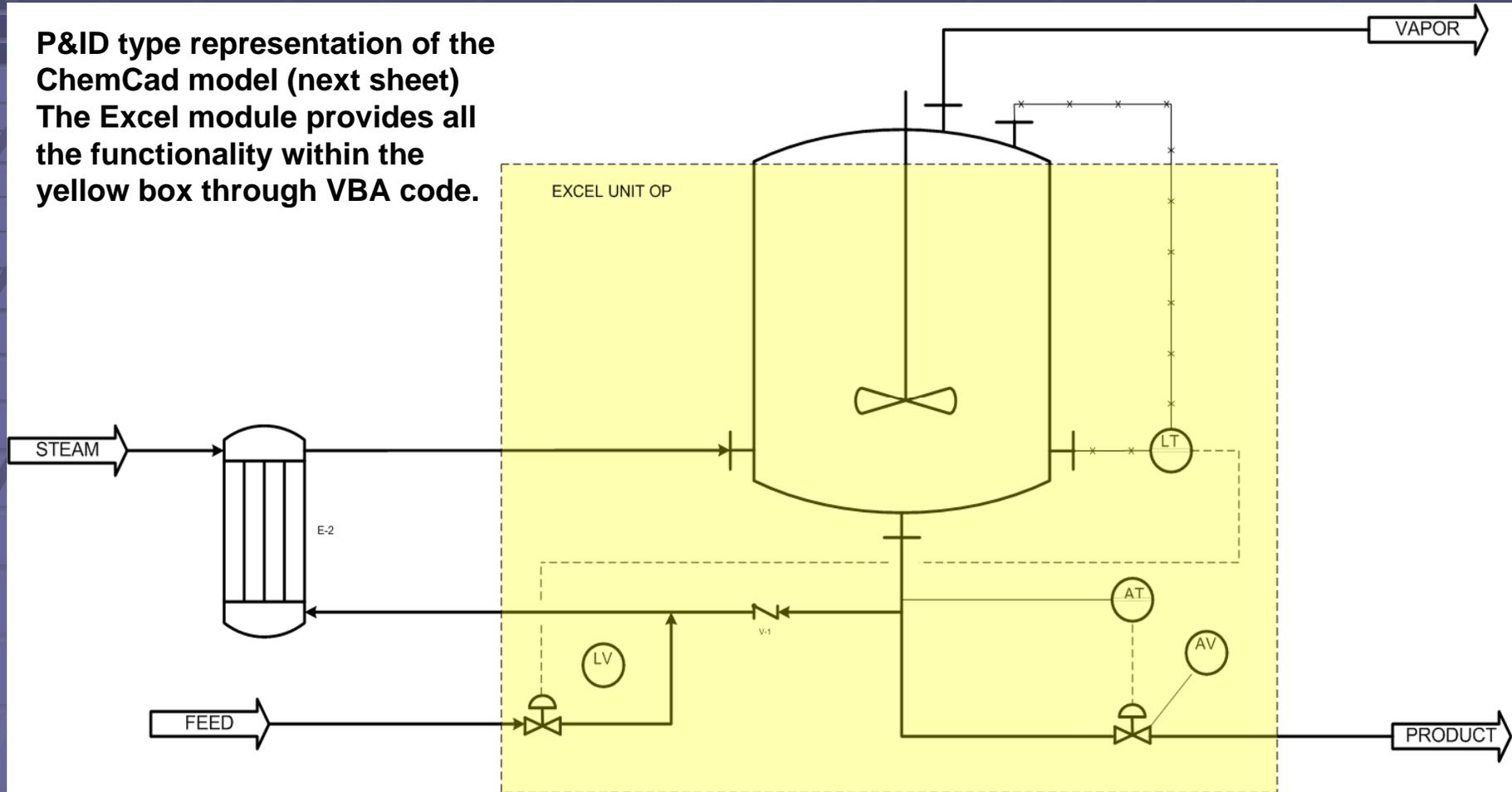
# Unsteady State Evaporation

## System Description

- A dynamic salt concentration evaporator utilizing an Excel unit operation with VBA within CC-SteadyState is modeled.
- The excel unit operation models two PID controllers and a 'batch' reactor (as depicted next sheet).
- The Excel module acts as a splitter and divider as part of the control functions above.
- Na salt concentration is calculated by the VBA code.
- The Excel module serves as a data logger for the results of each time step, displaying the results via an Excel graph.
- Recirculation flow rate is equivalent to level.

# Simple Evaporator P&ID

P&ID type representation of the ChemCad model (next sheet)  
The Excel module provides all the functionality within the yellow box through VBA code.



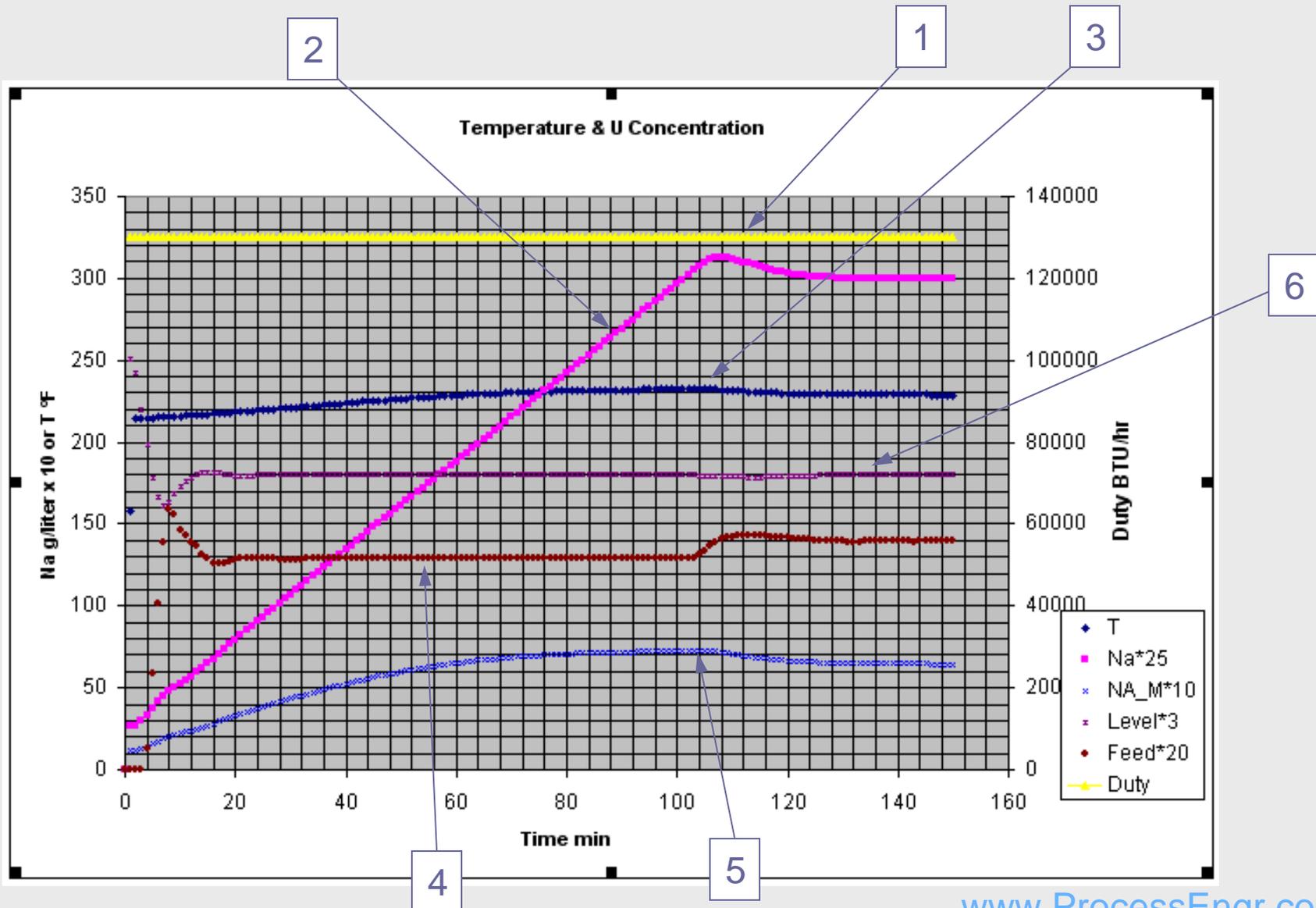


# Unsteady State Evaporation

## Summary of Simulation:

1. Feed starts to bring level to setpoint.
2. Cold inventory is heated in the thermosiphon reboiler and begins to boil.
3. Concentration of salt & acid increases as a result of evaporation of mostly water.
4. When the product controller setpoint salt concentration is eventually reached, the product withdrawal starts.
5. Level drops with product withdrawal and feed increases to make up the loss, maintaining the concentration at setpoint.
6. The system is now at steady state as long as feed can be maintained.
7. All of the above steps are controlled by the Excel module which is called by ChemCad once per iteration.

# Excel Output from Batch Run (see next slide for explanation)



# Explanation of Graph

Note: Output scaled to make graph readable.

One minute = one iteration of ChemCad simulation.

1. Exchanger Duty (constant)
2. Temperature – starts 70°F, but quickly brought up to evaporation temperature and then varies slightly with nitric acid concentration.
3. Sodium (salt) concentration – controlled by product removal - ramps to setpoint and levels with slight overshoot.
4. Feed rate - starts high to makeup low starting level, then levels off. Increases slightly as Na reaches specification and drawoff starts after about 2 hours.
5. Nitric acid concentration - starts low and increases with evaporation, but decreases as feed increases with product take off.
6. Level – starts empty, but quickly brought to steady state operation level by feed controller.

# Using CC-SteadyState to model unsteady state operations

- Time basis requires careful attention.
- Visual Basic knowledge required.
- VBA is very powerful when used with ChemCad; nearly every aspect of simulation can be controlled.
- Simulation can be fairly complex, but the method is best suited to simpler operations

# Excel Module vs. VB Server Methods

- The Excel module adds several steps to building the model.
- More control using the VB server method.
- Easier to run VB server (no switching applications)
- In a very brief test, the evaporator model with the Excel module ran 10x faster than the same code under VBA control.

# Controls

- Many models won't need them.
- Recommend direct calculation in VBA if possible.
- Could use CC steady state controller with VB server.
- Use ChemCad built-in PID control? Not sure.
- A custom PID controller in VBA can handle difficult situations with a fairly predictable amount of work, but it can be hard to tune, (but this is very cool & great entertainment for engineering geek types).

# Time considerations

- ChemCad only offers minutes, seconds or hours as time units.
- Native ChemCad (as accessed by VBA) has time units of hours only. If the VBA code does any time or rate calculations, it will be necessary to convert to the proper units.
- Great care is needed to maintain consistency.
- Any iteration time (other than hr, min, sec) is possible, but tracking the time will be completely up to the user.
- Each iteration within ChemCad is one time unit. If ChemCad time units of hr, min, or sec are used, tracking is easier, but still requires care and thought, especially for the VBA code.
- It is better to run too many iterations than too few, but the time units available are limited.

# In Summary

- System flow (per iteration or time period) is the equivalent of volume.
- The time increment per iteration requires considerable care.
- A PID controller can be quite powerful, but requires a certain level of complexity.
- Operating a dynamic simulation through steady state ChemCad is probably best handled through a VB server approach, but an Excel module may increase the speed of operation.