

# Simulation Best Practices & Common Mistakes



Chemstations™

*Engineering Advanced*

# Best Practices

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Start with good physical property data

Choose & validate your thermodynamic model

Build model one step at a time

Handle recycles with care

# How to determine if properties are good

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Operational data is great

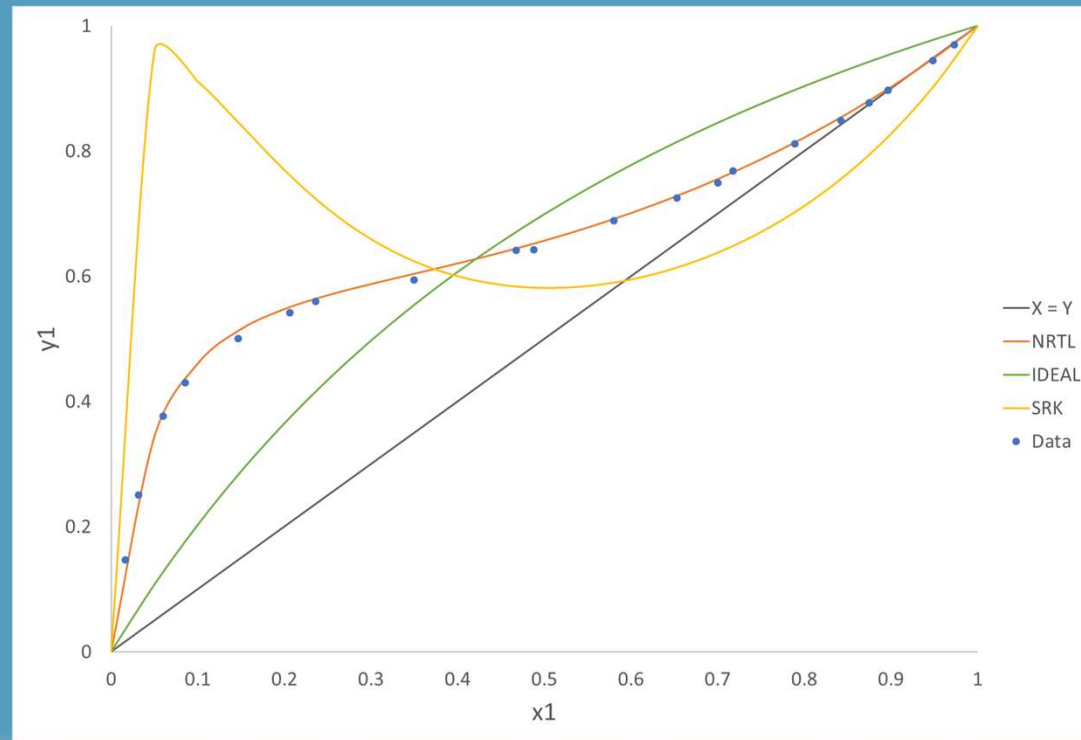
Pilot plant data is good

Lab data is ok

Literature data is... sometimes not bad

Predicted data is...brave

# Learn how to choose thermodynamics



# How do you choose your thermo model?

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Experience with thermo is necessary

Articles / books can teach you basics

Compare to data for important systems

# Validate your thermodynamic model

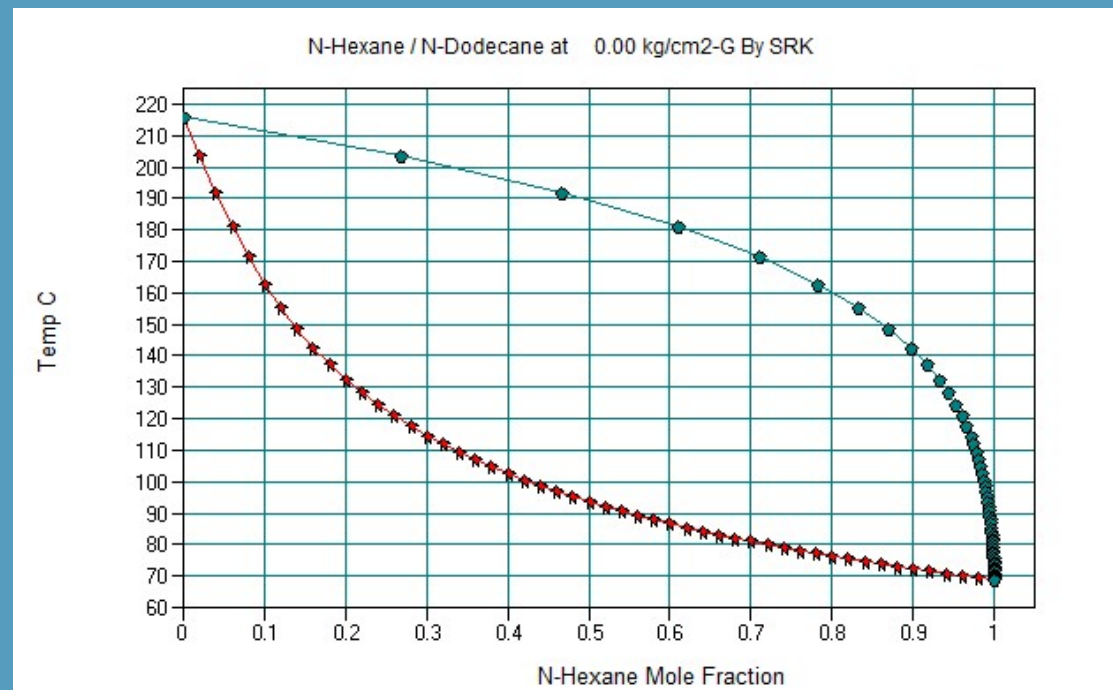
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Inspect TPxy diagrams

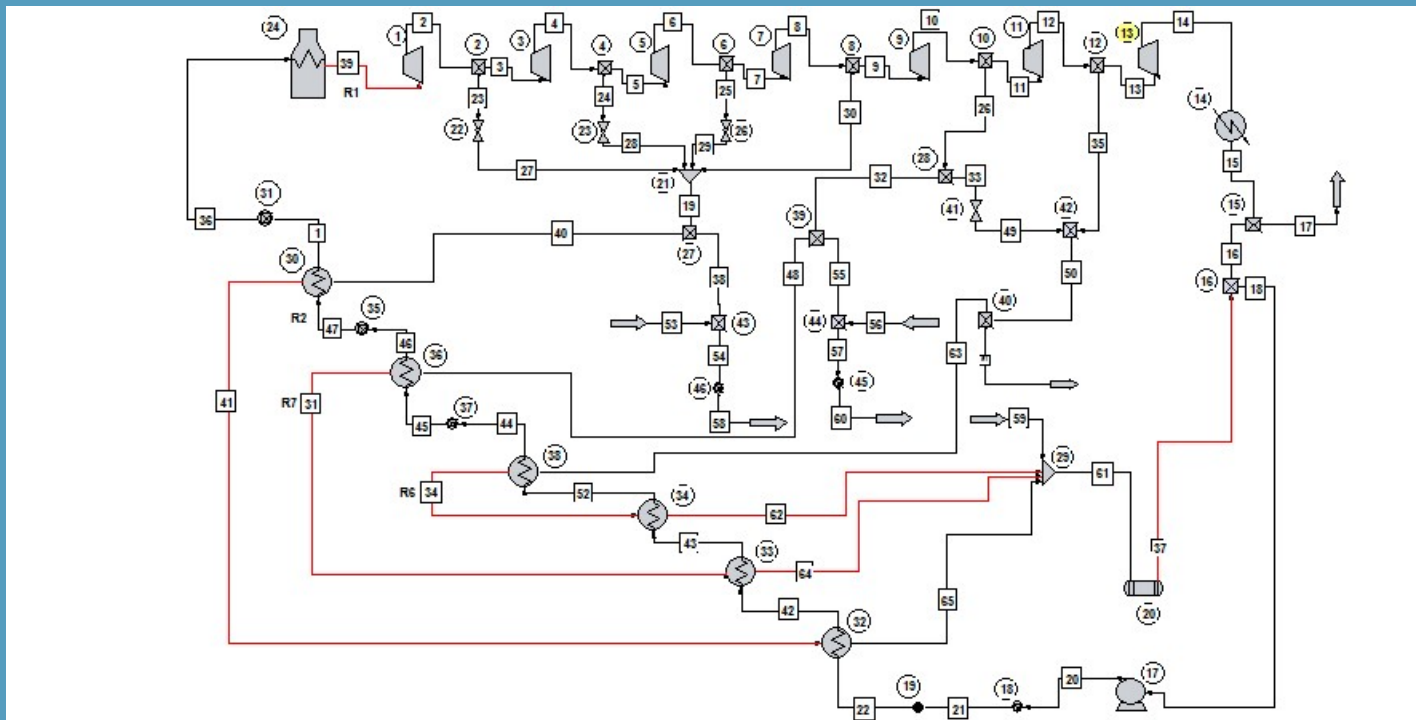
Run some flash calculations & inspect results

Have a qualitative idea of what the phase separation will look like

# Learn how to read Txy, Pxy, Txx, xy diagrams



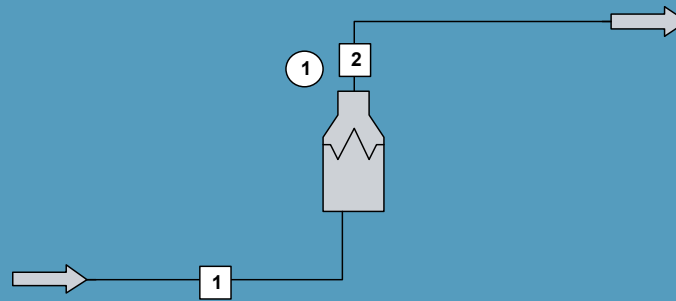
# One step at a time!





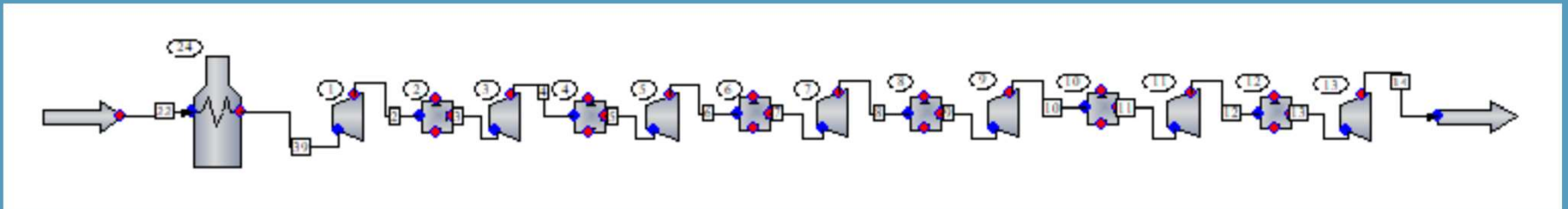
# Start simple

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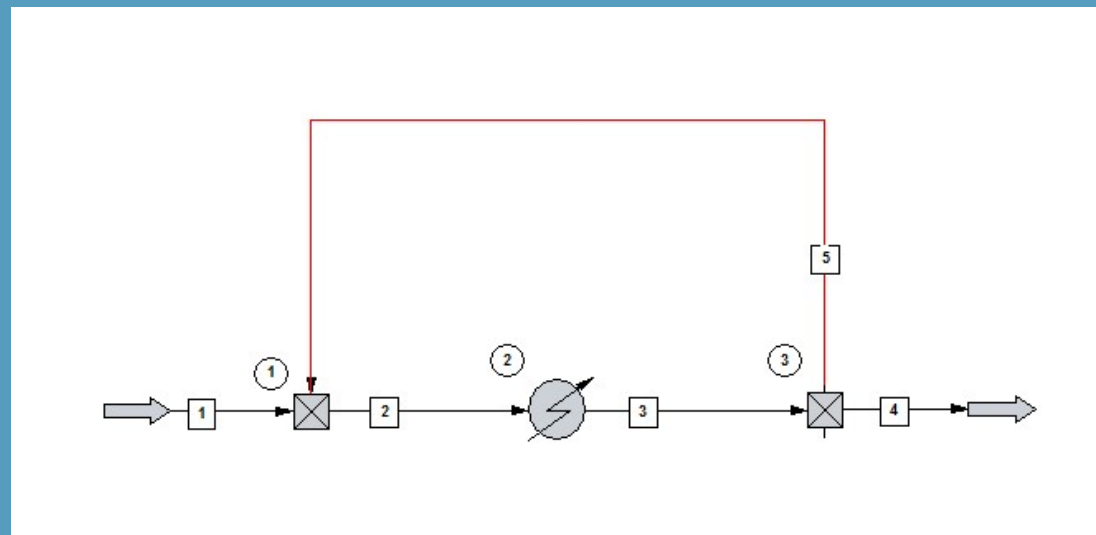


# Add piece-by-piece & converge at each step

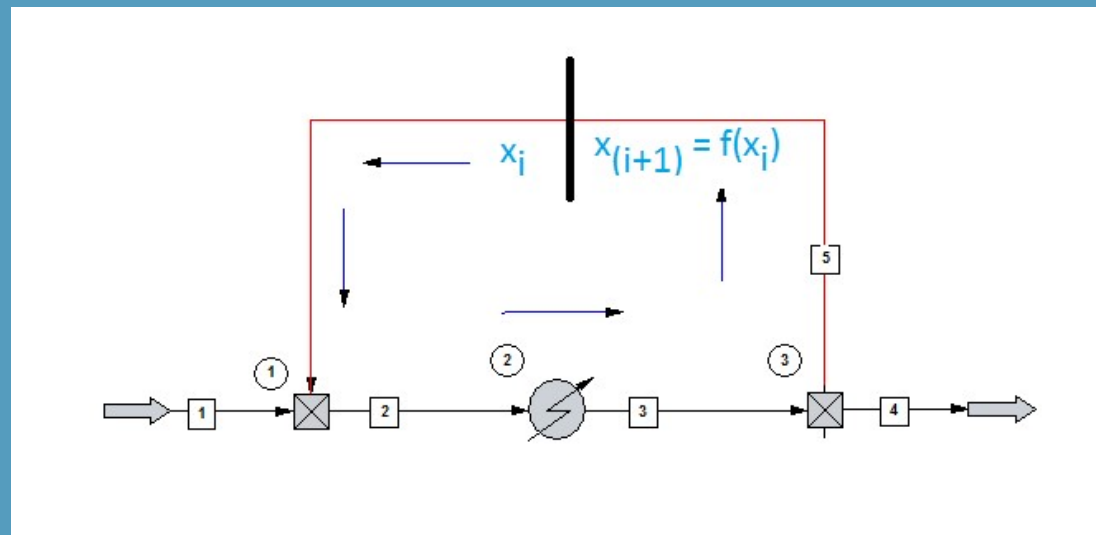
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# Handle recycles with care

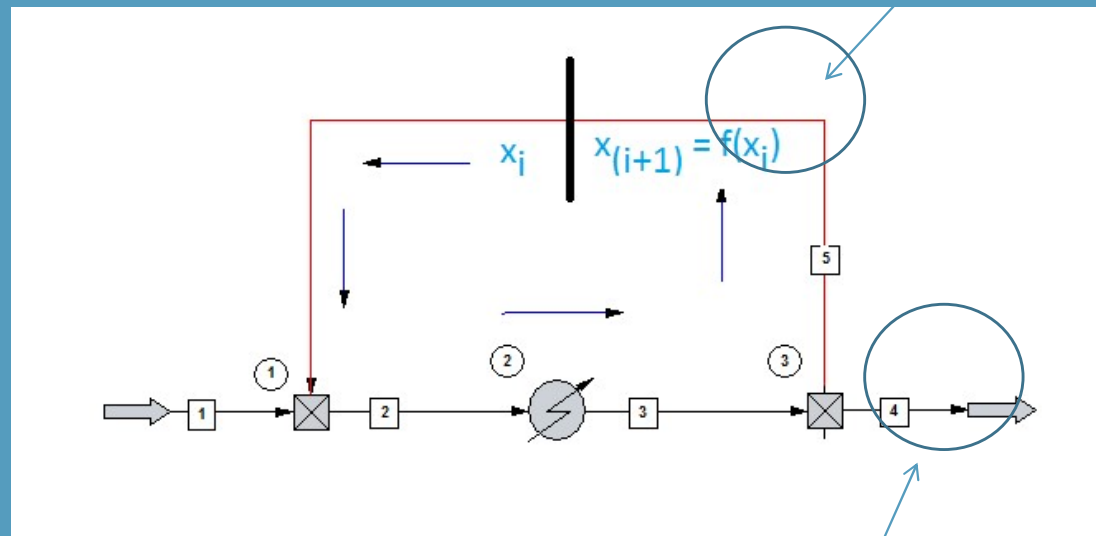


# Calculations get more complicated



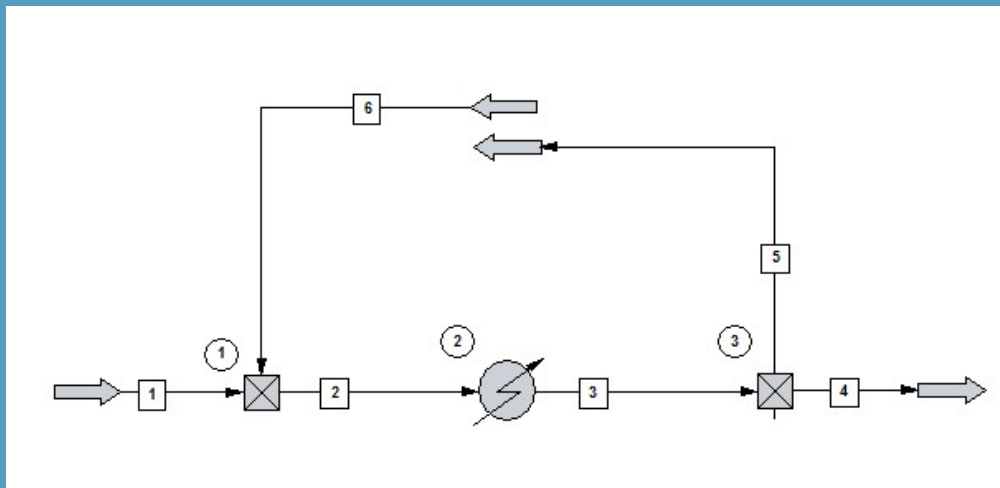
# Put in a good initial estimate

Specify this flow rate to stabilize calculations!



Let the simulator calculate this flowrate

# Start off with loop open to get estimate



# Common Mistakes

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## Matching plant data

- How accurate are the measuring devices? When were they last calibrated?
- Were all measurements taken at same steady state conditions?
- Are you ignoring trace chemicals?
- Neglecting to examine different conditions (cooling water can average 90°F in Houston summer)

## Simulators get played like a video game

- Converged doesn't necessarily mean correct

# Common Mistakes

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## Understand your process before modeling

If you don't know what you're doing, you'll get the wrong answer

## These are tools; you are the engineer

Garbage in = garbage out

Use engineering judgment, not necessarily default options



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