KM 331 PROSES BENZETİM PROGRAMLARI
DERS NOTLARI [1-4]

Kaynaklar

1. Chemcad User Guide and Tutorial, Chemstations, Inc. Version 6.1.
2. Aspen Technology, Inc., Apsen HYSYS ® Version 7.
3. ChemCad Eğitim Notları , Chemstations, Inc- Houston,TX,USA.
4. A Guide for Getting Started in Aspen HYSYS
   Dinu Ajikutira, Sr. Director, Engineering Product Marketing, Aspen Technology, Inc.

ChemCad Paket Programına Giriş

- 1984: professors develop first PC based process simulator; sell technology to McGraw Hill
- 1988: Chemstations purchases ownership and begins marketing CHEMCAD.
- 1992-1999: Chemstations launches CC-THERM, CC-BATCH, CC-ReACS, and CC-DCOLUMN.
- 2000: Chemstations sells to 1000th customer
- 2006: Chemstations builds an OPC Server interface into CHEMCAD

What does a process simulator do?

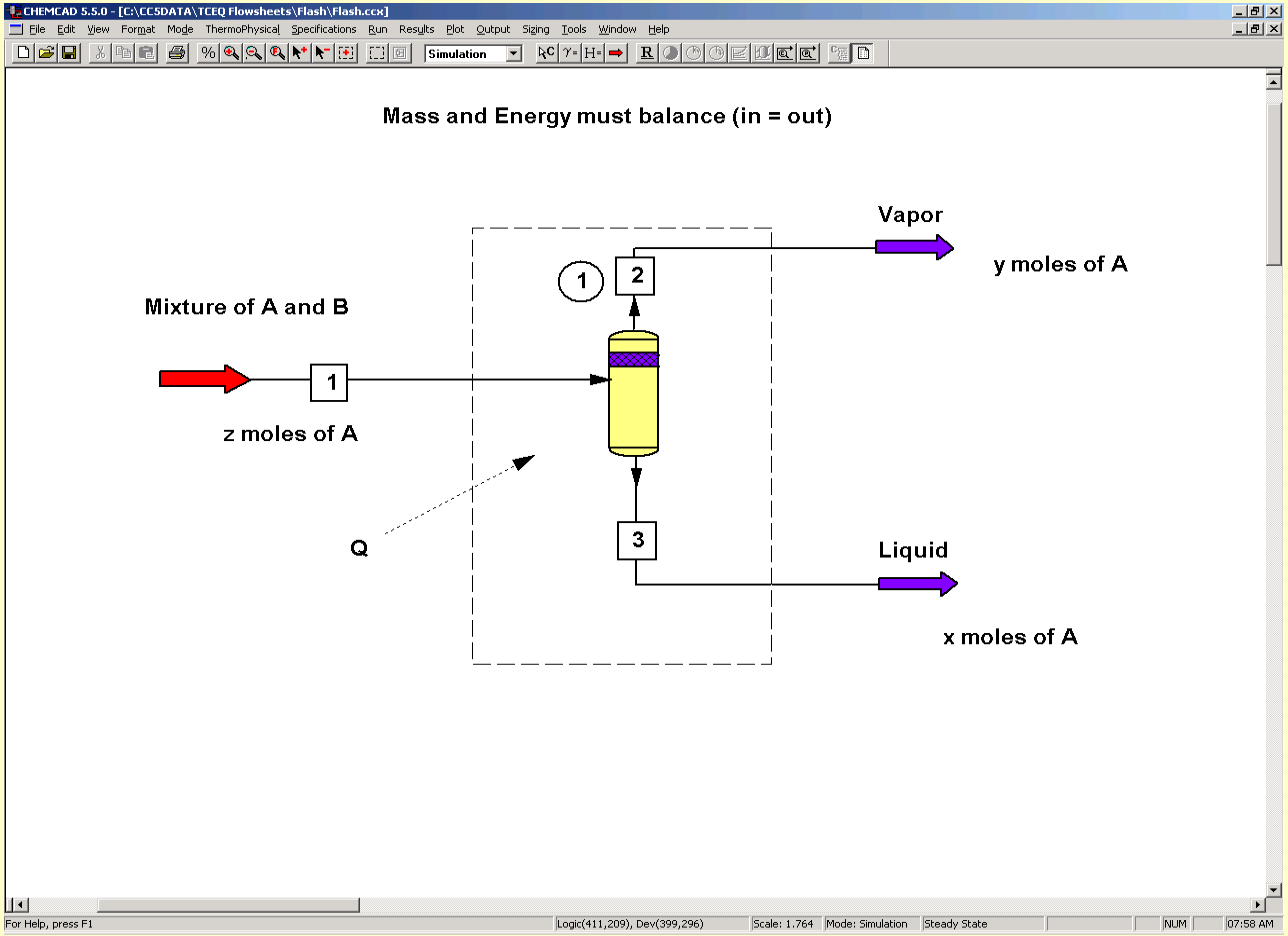
- heat and mass balances around unit operations
- calculation of what happens with vapor and liquid in unit operations
- Process simulators have databanks of transport properties of chemicals, thermodynamic models for vapor liquid equilibria, and models for common unit operations

  If I have 10 lbs of water, 2 lbs of nitrogen, and 1 lb of toluene and I add heat...what is the vapor composition? What is the temperature?

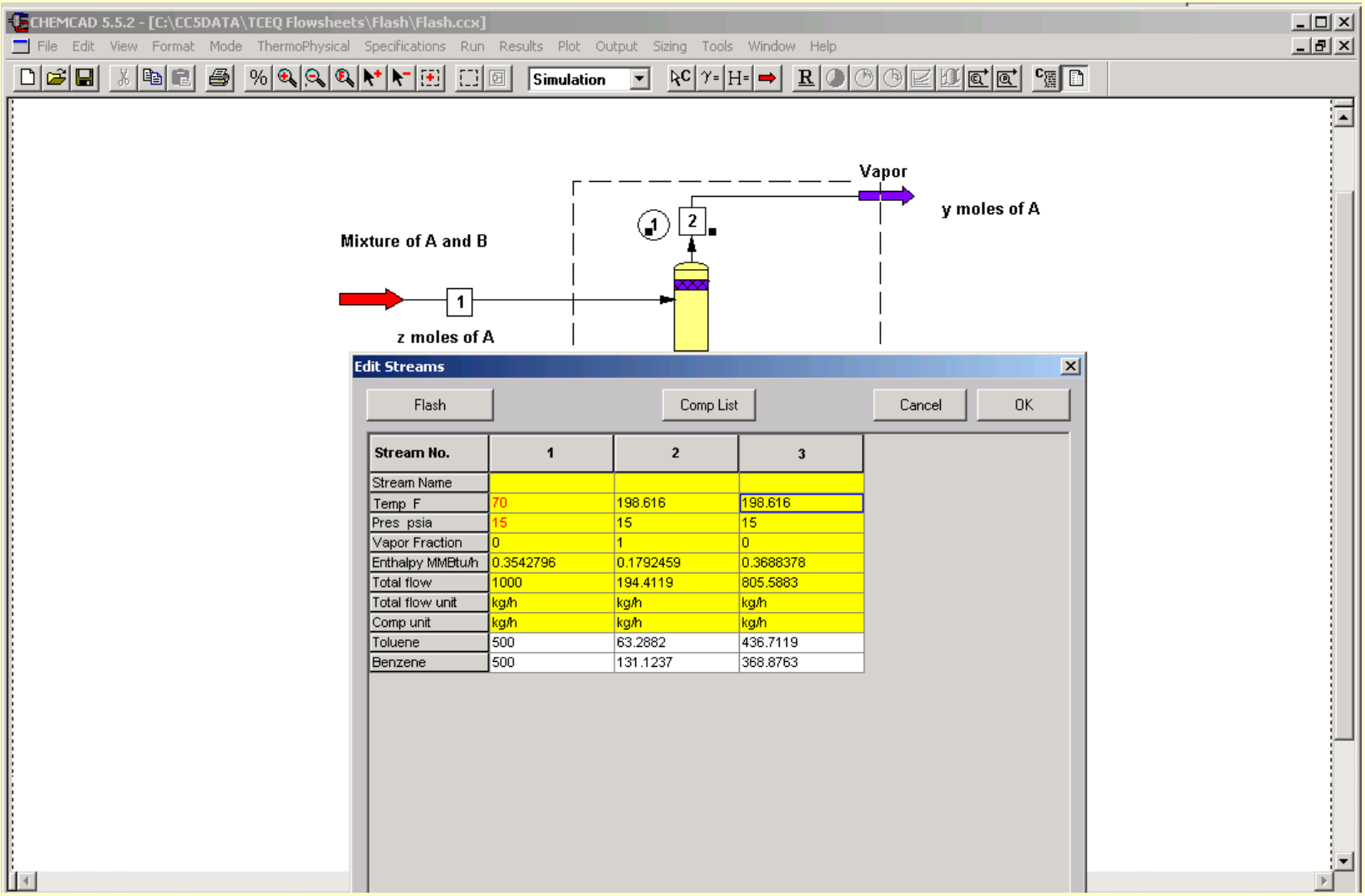
Components of a simulator

- Chemical database for calculating properties (Cp=f(A,B,C,D,T)
- Unit operation models (Q=U*A*LMTD)
- Thermodynamic package to calculate VLE (y_i*P = x_i*P_i^{sat})
- Graphic User Interface for flowsheeting
- Report tools

Mass and Energy balance

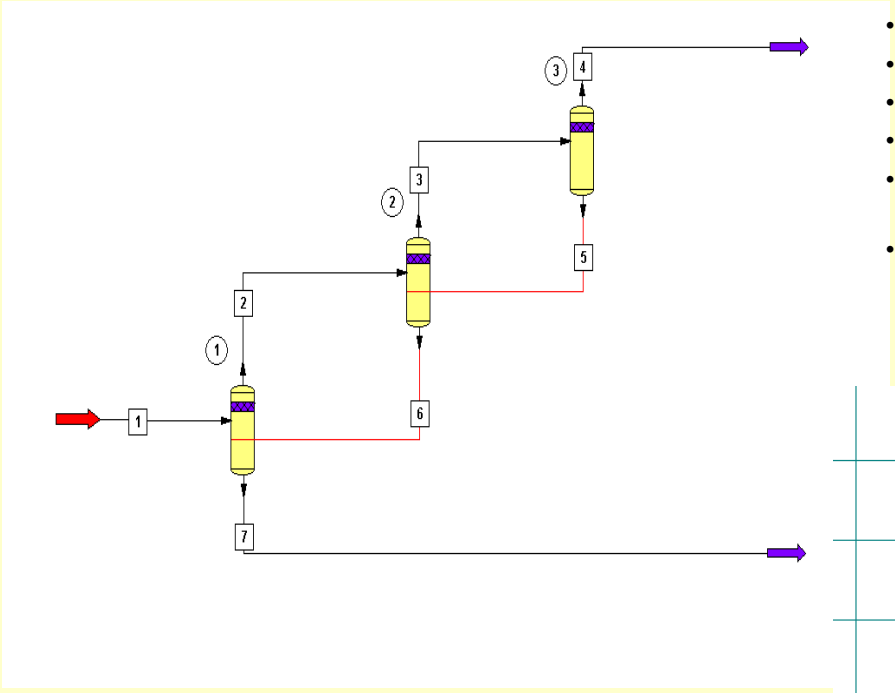


Thermo II: flash calculation



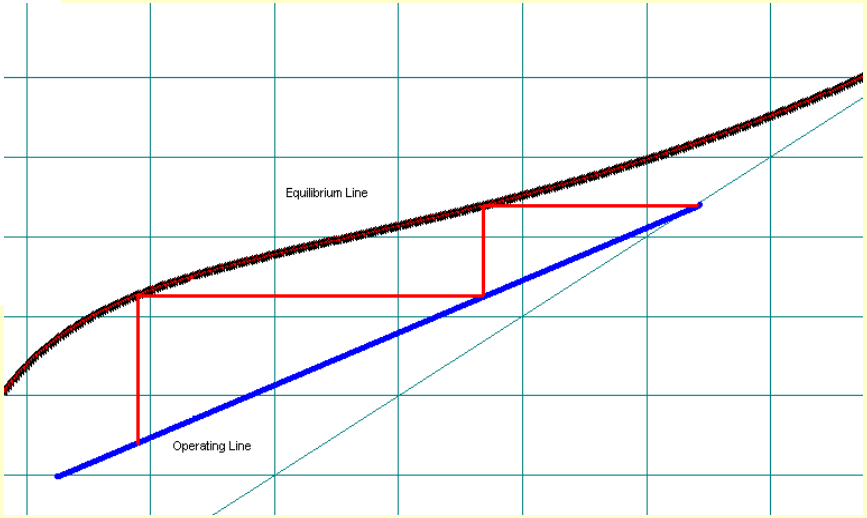
Stream No.	1	2	3
Stream Name			
Temp F	70	198.616	198.616
Pres psia	15	15	15
Vapor Fraction	0	1	0
Enthalpy MMBtu/h	0.3542796	0.1792459	0.3688378
Total flow	1000	194.4119	805.5883
Total flow unit	kg/h	kg/h	kg/h
Comp unit	kg/h	kg/h	kg/h
Toluene	500	63.2882	436.7119
Benzene	500	131.1237	368.8763

Unitops: Stepwise Distillation



- To derive the operating line equation, perform a material balance for the more volatile component:
- $V_{n+1} y_{n+1} = L_n x_n + D x_D$
-
- Assume constant molal overflow;
- $V_{n+1} = V_n = ... = V$
- $L_n = L_{n-1} = ... = L$
-

  The rectifying operating line thus becomes: $V y_{n+1} = L x_n + D x_D$
- Now, from $V_{n+1} = L_n + D$, we have $V = L + D$



What do engineers do with process simulators?

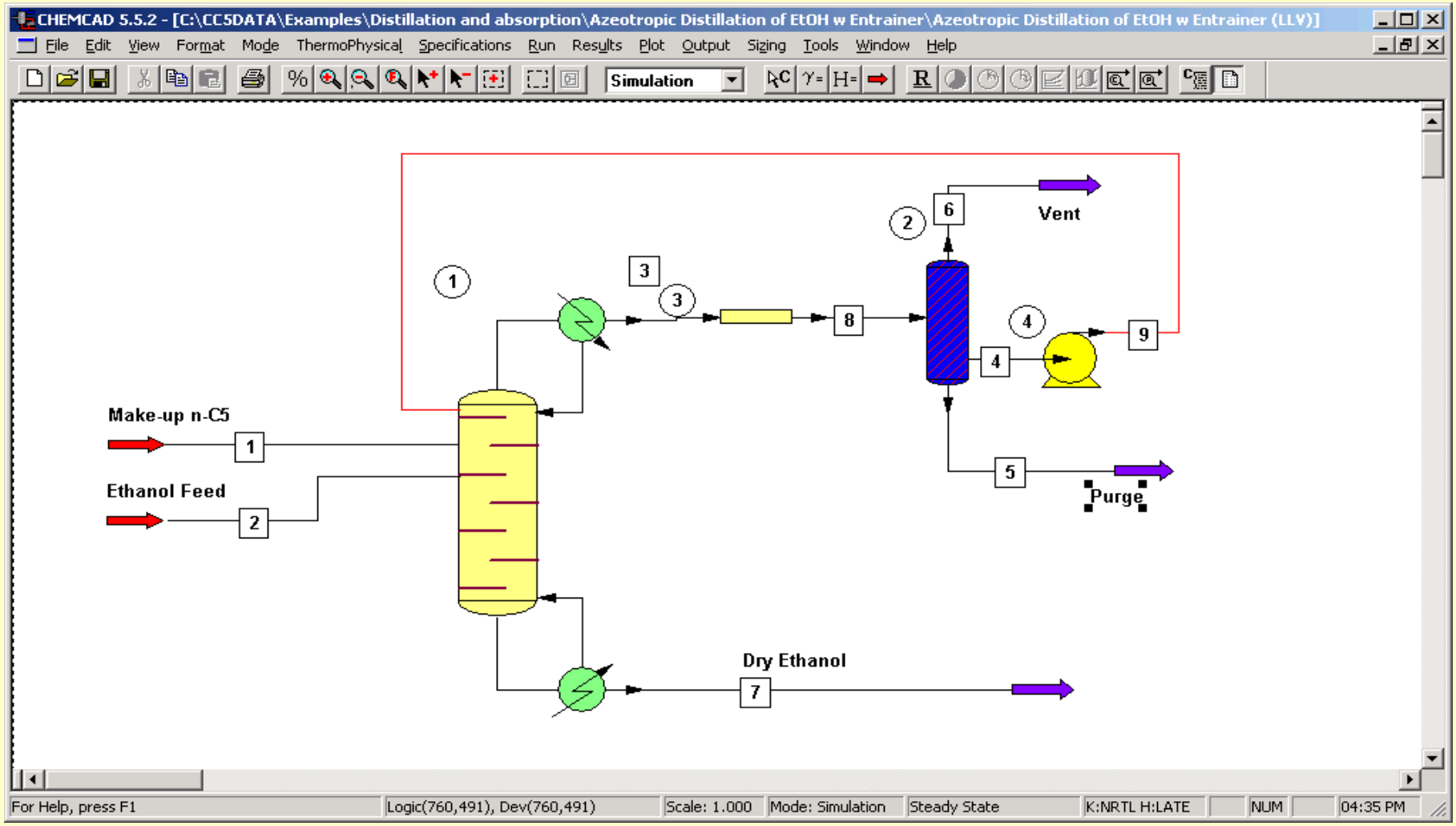
- Model existing facilities
- Design new facilities
- Connect to control system for monitoring / control
- Study relief devices and piping networks
- Related calculations (unit conversions, transport properties)

Designing new process

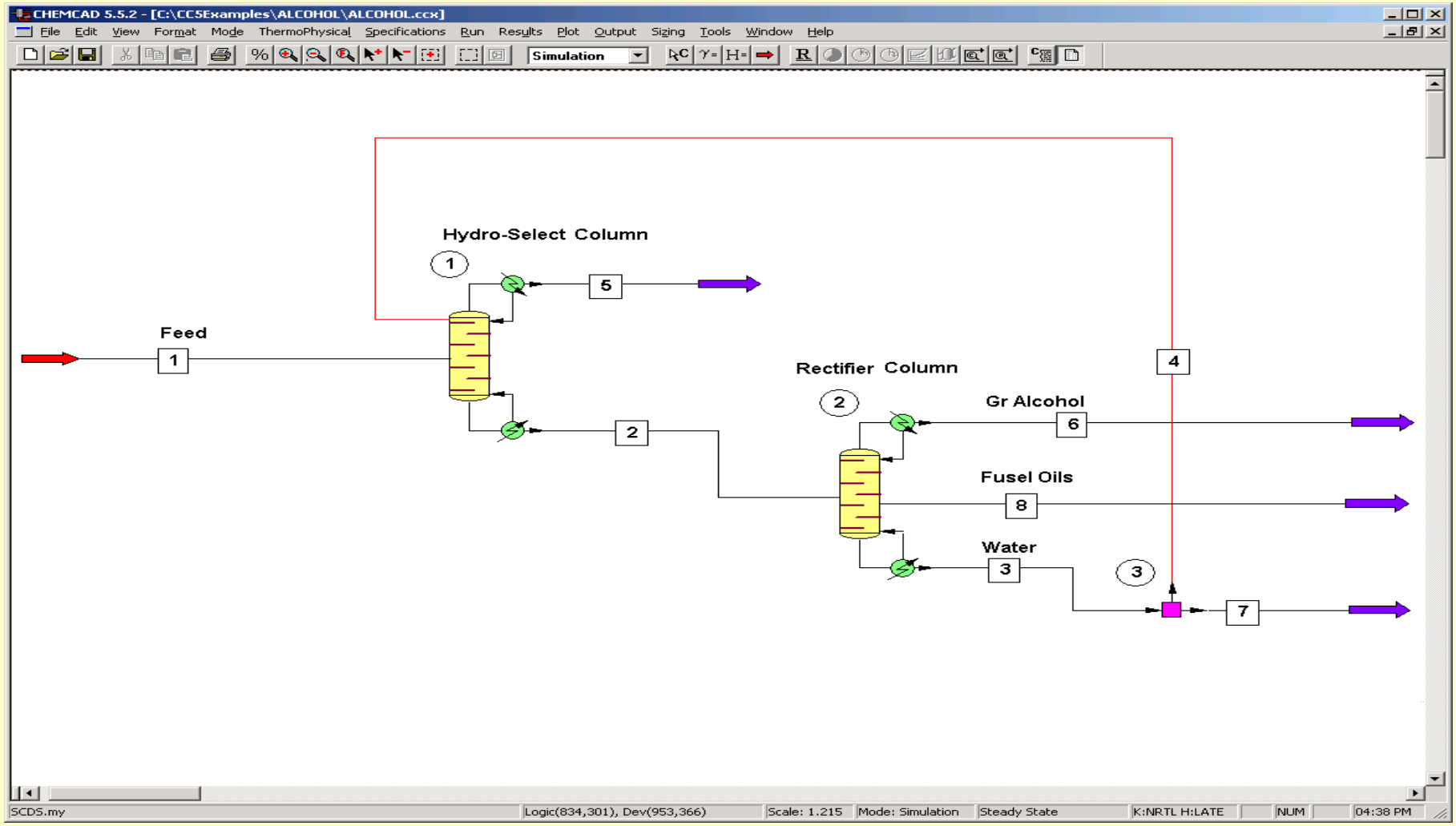
- Determine if process is feasible
- Look for problem areas
- Try different configurations before you build

- *In the real world, you apply heat and measure the result*
- In simulation, you specify the result you want, and calculate the heat you need

Ethanol by entrainment



Ethanol by pressure swing



Process Simulations Solutions