Computational Methods of Analysis and Design

Laboratory Exercises

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Lab 5

Recycle with simulator
Example
  – Ammonia production

Structure of the exercise
  – Flowsheet
  – Test different solution methods
  – Convergence comparison
  – Optimization of Design parameters
  – Sensitivity analysis
Flowsheet

N2  100 kmol/hr
H2  300 kmol/hr
CO2 1 kmol/hr

N2  1.2 kmol/hr
H2  3.7 kmol/hr
NH3 197.5 kmol/hr
CO2  1 kmol/hr
Feed
- Initial feed conditions 80°F και 300 psia
- Feed:
  • Nitrogen (100 kmol/hr ),
  • Hydrogen (300 kmol/hr ) and
  • A small amount of CO2 (1 kmol/hr ) from hydrogen production process
- Feed is compressed isentropically at 4000 psi

Mixing of feed and recycle
- Feed is mixed with recycle and heated at reactors temperature (900°F, 4000 psi)
Data

Reactor
- Temperature 900°F and pressure drop 30 psi
- Feed composition is 3:1 α
- For composition at chemical equilibrium: RGibbs.
- Output stream is cooled at 80°F
Flash vessel
- $T = 80^\circ\text{F}$
- Vapor phase is recycled after being recompressed

Recycle and purge
- Vapor phase is recycled except from 0.01% that is purged
- Before recycle the gas is compressed isentropically at 4000 psia

Thermo-dynamic method PSRK
Simulation

Select tear stream 10

Try

- Wegstein
- Broyden
- Newton
- Direct substitution

Compare after 30 iterations

Which is simpler and which has the best results

Test different tear stream and number of iterations
AS P E N
Ammonia production flowsheet

A. B7, B8 (Compr)
B. B5 (Mixer)
Γ. B1 (RGibbs)
Δ. HX B3, B4
E. Separation B2 (Flash)
ΣΤ. Stream split B6 (Split)
Components
PSRK
& input stream
Heat exchangers
Mixer and splitter
Separation
Tear stream 10 (30 Iterations)
Change convergence method – for 30 iterations

Data → Convergence → Conv Options
Default methods: Broyden, Direct, Newton, Wegstein

- Broyden OK,
- Direct no convergence,
- Newton OK,
- Wegstein no convergence
Tear stream 3 (30 Iterations)
Change convergence method – for 30 iterations

Data → Convergence → Conv Options
Default methods: Broyden, Direct, Newton, Wegstein

Broyden OK,
Direct no convergence,
Newton OK,
Wegstein no convergence
More iterations

Direct no convergence 30 iter and 10^-4 tear tolerance,
Wegstein no convergence 30 iter and 10^-4 tear tolerance

Direct 2000 iter, & 10^-6 tear tolerance OK
Wegstein 1000 iter, & 10^-6 tear tolerance OK

->Simulation calculations completed ...

*** No Warnings were issued during Input Translation ***

*** No Errors or Warnings were issued during Simulation ***