Modeling and simulation of Multicomponent Distillation systems

Objective:

Given the feed composition and feed conditions along with the operating and design parameters of the distillation column, get the steady state temperature and composition profiles along the column. Also get the plot of top and bottom stage temperatures and compositions versus time (dynamic behavior of the column) for a given initial condition. Following are the different types of models and the developed code is expected to be based on the suggested modeling strategies. Compare the results obtained with different models and also with the published results, if any.

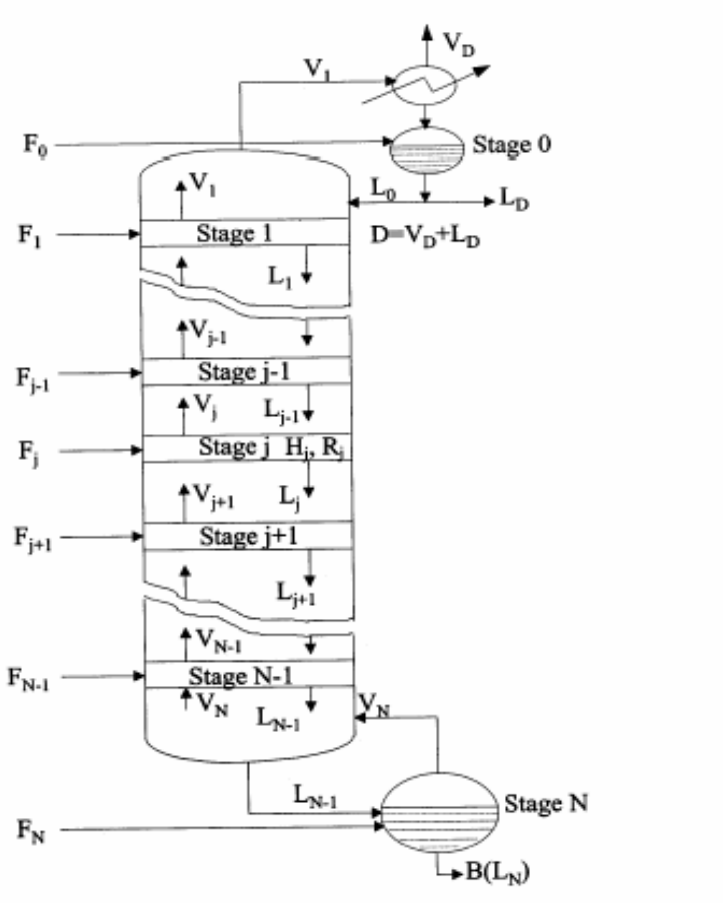

Figure 1:Generalised distillation column

Models:

1. Equilibrium stage model with constant molar overflows with ideal or non-ideal liquid phase.
2. Rigorous equilibrium stage model including energy balance and excluding stage efficiency factor. The model should be with and without constant molar holdup & energy holdup.
3. Rigorous equilibrium stage model including energy balance and including stage efficiency factor.
4. Non-Equilibrium stage model :
    - Conservation equations are written for each phase separately.
    - The conservation equations for each phase are linked by material balance around the interface, i.e. inter-phase mass transfer rates are included in the balance equations.
    - Similarly the energy balance for each stage is written by splitting into two parts one for each phase, each containing a term for the rate of energy transfer across the phase interface.

Assumptions and requirements:

The developed code should satisfy following conditions:

1. Multi component system (components greater than or equal to 3)
2. Applicable to reactive and non-reactive distillation by changing suitable parameters.
3. Capability of feed input at any stage including reboiler and condenser, with any feed condition.
4. Condenser can be total as well as partial.
5. Liquid phase non-ideality may be included using any appropriate thermodynamic model (e.g. Uniquac, NRTL, Wilson etc), with ideal vapour phase.
6. Model may accommodate constant and non-constant molar liquid holdups and energy holdups, with negligible vapour holdups.

7. Model should be formulated with and without stage efficiencies.
8. Adiabatic column can be assumed (no heat loss to the surrounding).
9. Reaction may be assumed to take place in liquid phase in case of reactive distillation.
10. Pressure variation along the column may be accommodated.

Referances:

1. Seader J.D. and Henlay E.J.. Separation Process principles. New York.
2. Taylor R and Krishna R " Modeling of Homogeneous and heterogeneous Reactive distillation, Chapter-9, Reactive Distillation : Status and Future Directions, Book by Kai Sundmacher and Achim Kienle, New York :Wiley
3. Taylor R and Krishna R (2000), Modeling Reactive Distillation, Review, Chemical Engineering science, (55) , 5183-5229.
4. Taylor R and Krishna R (1993), Multicomponent Mass Transfer, New York : Wiley.
5. Chen, F., Robert S. Huss, F. Malone, Michael F. Doherty (2000), Simulation of kinetic effects in reactive distillation, comp & chem. Eng. 24, 2457-2472.

Note:

1. Select any convenient system for the application of above mentioned modeling and simulation strategies.
2. Use any programming language to implement the solution strategies of the model equations, like MATLAB, C, C++ etc. Standard FORTRAN packages can also be used like LSODE(ODE solver), RADAU5 (DAE solver) etc.