During the last decade, there has been a rapid upturn of interest in reactive distillation. The chemical process industry recognizes the favorable economics of carrying out reaction simultaneously with distillation for certain systems and many new processes are being built based on this technology.

In this work, equations of a reactive distillation column were described and derived for a multi-component system. New sets of transformed composition variables were defined. These sets allow for the computation of the concentration profiles along the column and therefore a simple relationship between the reflux and reboil ratios. The system was assumed to be in both chemical and vapor-liquid equilibria. The new sets of transformed composition also help to eliminate the source term accounting for chemical reaction in the conservation equations; in other words, the transformed variables provide a way of reducing the dimensionality consistent with the Gibbs phase rule.

The complexity of the equations characterizing reactive distillation systems can be diminished by ensuring that, in the case of complex reacting systems, only the very minimum of reactions are considered. So, in the complex reactions where there are a myriad of single reactions to be considered, there is need to ensure that only independent set of reactions are considered. Therefore, there is need to consider how to achieve this objective. A computer-assisted procedure was developed for the determination of independent elementary steps in reactive schemes. The procedure facilitates the rapid reduction of large mechanistic and molecular reaction schemes into independent sets of reactions. The procedure was tested on some examples taken from the pyrolysis literature. These are the mechanisms for n-butane pyrolysis, cyclohexane pyrolysis' and some selected reactions of the mechanistic and molecular steps in n-heptane pyrolysis.

Although, the reaction system considered in this work is not complex enough to warrant the use of this concept of independent reaction, it is obvious that this topic is essential in any general kinetic schemes. For future developments of reactive distillation applicable to any
reactive system, simple or complex, the role of the concept by independent reaction is assured.

Reactive distillation, a new separation process was employed to separate meta – and para – xylene mixture. A third component, di-tertiary butyl benzene was intentionally introduced (as a reactive entrainer) to react with m- xylene. The alkylation reaction complex, tertiary-butyl-m-xylene on reacting with more benzene liberated the m-xylene in another reaction step. The phase diagram in terms of the new composition variables was constructed. The residue curve maps in the transformed composition variables for the reactive mixture at equilibrium provide information on the feasibility of separation and even column sequencing of a desired separation.

The separation of C8 close boiling aromatic compounds- a more complex system, using reactive distillation was done. A separation based on alkylation, separation of the alkylated products and their subsequent dealkylation and the final separation produced the high grade pure xylenes and ethylbenzene compounds. Meta, para, ortho – xylene and ethylbenzene form a close boiling mixture and they are isomers of C8 compound. A fifth component, di-tertiary butyl benzene, was intentionally introduced into the system (as a reactive entrainer) to react with o- xylene and ethylbenzene with the aid of the highly selective iron chloride (FeCl3 ) catalyst in the first column. The separated alkylated complex, tertiary- butyl-o-xylene and tertiary- butyl-ethylbenzene, liberated the o-xylene and ethylbenzene in another reaction step on reacting with more benzene. AlCl3 catalyst allows the reactive entrainer to react with m- xylene to form a complex : tertiary- butyl-m-xylene. This complex was separated and dealkylated in another step. The new variables represent the surfaces embedded within the mole fraction coordinate space in a simpler way, thus giving an easier visualization of the diagrams of the combined phase and chemical equilibria. This made the determination of the feasibility and sequencing of the distillation columns easier.