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# Application of e-KT-UNIFAC Model for Improved and Innovative Design of Biphasic Reacting Systems

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## Abstract

Biphasic reacting systems have a broad range of application in chemical, pharmaceutical, and agro-bio industries. The systems contain two immiscible liquid phases, in which reactants and catalysts (including also biocatalysts and enzymes) can exist in different liquid phases, allowing novel synthesis paths, higher yield, and faster reaction rate, as well as, making the separation tasks easier by manipulating process condition after reaction. A mathematical model which collectively describe reactions, mass transfer, and equilibrium of heterogeneous species is constructed with the biphasic reacting systems modelling framework [1]. It can be a powerful tool for an improves and innovative design of the systems.

To handle the complexity of the system, the system is divided into sub-systems of binary species which require an appropriate thermodynamic model to predict the partition and equilibrium of the involved species. In the earlier models, different thermodynamic models are use for each sub-systems, which inevitably increase the complexity and uncertainty of the model. Recently, a predictive electrolyte model based on group contribution method (e-KT-UNIFAC) [2] has been developed. This new model has been successfully applied for alkali-halide salts in aqueous and mixed solvent systems and has the capability to predict the partitioning and equilibrium of electrolyte and non-electrolyte systems and also has the potential to accommodate a wide range of reaction systems and solvents.

In this work, a case study involving the production of 5-hydroxymethylfurfural (HMF) from biomass in a biphasic system is used to show application of the framework. The implementation of the model for improved and innovative design of system will be demonstrated.

## References

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