



## Molecular Tracking: An Alternative Computer-Aided Concept for Multi-Component Distillation Column Design

Nazemzadeh, Nima; Udugama, Isuru A.; Abildskov, Jens; Mansouri, Seyed Soheil

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# Molecular Tracking: An Alternative Computer-Aided Concept for Multi-Component Distillation Column Design

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## Abstract

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In this work a new design methodology for distillation columns is proposed based on the concept of molecular tracking. This is a novel computer-aided design tool for distillation processes. Molecular Tracking methodology works by tracking one single molecule at a given time from the feed location to outlet streams of column (distillate, bottom and probable side streams). The method is based on a probability function, which is highly correlated with system thermodynamics and operations such that it produces a random pathway for each molecule that is then visualized. Combining these “random pathways” allows generating a detailed visualization of the internal movement of components within the column. In comparison to the traditional approach design methodologies and corresponding simulations, molecular tracking approach provides a number of benefits such as intuitive visualization and the ease of reconfiguration with respect to additions such as side-draws as well as divided wall, which are becoming increasingly common.

This study first analyzes in detail the influence of thermodynamic properties and operational conditions on molecular tracking by demonstrating the concept on a simple binary distillation unit. This is followed by an industrial case study of a high purity methanol distillation unit consisting multi-component methanol and water feed with trace levels of ethanol. In this case study, molecular tracking is employed to find the optimal location of the column side draw. The analysis is based on thermodynamic and operational information gathered column with classical column configuration (only a distillate and bottoms). The generated results are then compared with results obtained from a validated process simulation and industrial observations.

Finally, this work will discuss in detail the pros and cons of the concept of molecular tracking, its coordinates in relation to existing computer-aided process design tools and the future developments required to exploit in full its potential.

## Authors

Follow Us: [Nima Nazemzadeh](#)

Politecnico di Milano

File [Isuru A. Udugama](#)

Technical University of Denmark

[Jens Abildskov](#)

Technical University of Denmark

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[Seyed Soheil Mansouri](#)

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*Abdallah Alshammari, CHE, KFUPM, DHahran, Saudi Arabia and Farrukh Ilyas Abid, CHE, KFUPM, DHAHRAN, Saudi Arabia*

**Optimal Design and Operation of Four-Product Dividing-Wall (Kaibel) Distillation Column**

Abdallah Alshammari\* & Farrukh Ilyas Abid  
alshammari@kfupm.edu.sa