## Invited Lecture IL 04

# Performance improvement on dynamic simulation for high pressure polyethylene synthesis by PC-SAFT

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Key Word (3 words)

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Abstract (less than 300 words)

High pressure polyethylene synthesis process requires advanced thermodynamic models such as PC-SAFT, and it is challenging to satisfy both computational reliability and performance, which are critical for dynamic simulation. In this work, two new computational techniques were developed and applied in our customer's projects. The first one is to improve the reliability by identifying a unique tangent point of the equation of state (EOS) [1]. The second one is to extend the squeeze theorem to functionals for performance improvement.

For any EOS there exists one tangent point which separates the vapor and liquid densities. With such tangent point, the computational effort solving the density roots can be significantly reduced. It also provides guarantee to avoid fake density root, so that complicated model like PC-SAFT can be reliably solved in high pressure region. Squeeze theorem states that if $f_L(x) \leq f(x) \leq f_U(x)$ for all $x$, then at some values of $x$ (references) all three functions are equal. Such theorem can be extended into functionals $g_L(X_L)$ and $g_U(X_U)$ which replace $f_L(x)$ and $f_U(x)$ where both $X_L$ and $X_U$ are functions of $x$. Within a neighborhood of a reference $(x \pm dx)$, the "squeeze"-relation still holds by those functionals, and the complicated $f(x)$ can be simplified by its first order Taylor expansion. The gap of the functionals would then be monitored to trigger necessary recalculation of $f(x)$ if value of $x$ is moving away from the reference neighborhood. We call this squeeze functional as "super-linear" approach.

Both techniques are generally applicable to any EOS model. To keep the generality and best protect our customer's confidentiality, examples were extracted and generalized from projects as vapor-liquid phase equilibrium problems. The results were compared with literature data. Performance improvement by the squeeze functional were observed with double to triple magnitudes faster than benchmark results without using it.

References

[1] G. Xu, N. Gerek Ince, Tangent Point Approach in Reliably Solving the Density Roots for PC-SAFT Equation of State, J. Chem Eng. Data 2020, 65, 12, 5643-5653