

Formula 1

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Formula 2

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Formula 3

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Detailed Explanation

Residual properties quantify the deviation of real fluid behavior from ideal-gas behavior at the same temperature, pressure, and composition. The workbook provides a rigorous, step-by-step framework for deriving these properties from cubic equations of state (CEOS), specifically PR and SRK, which are widely used in chemical process design and simulation due to their accuracy for nonpolar and moderately polar compounds. Each derivation begins with the fundamental residual property definition—e.g., $H^R = H - H^{ig}$ —and applies Maxwell relations and the thermodynamic network to express departures in terms of integrals involving $(\partial P/\partial T)_V$ and $(\partial P/\partial V)_T$. The workbook explicitly demonstrates variable substitution (e.g., using reduced or dimensionless forms), integration limits (from infinite volume to molar volume V), and handling of temperature-dependent attraction parameters $a(T)$ for PR/SRK). It also addresses numerical robustness—such as root selection for saturated phases, cubic root discrimination, and handling of metastable states—making it both a teaching tool and a reference for implementing custom property packages in equation-of-state-based simulators like Aspen Plus or open-source alternatives (e.g., Thermo, CoolProp).

Key Components

#	Component
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1	Analytical derivation templates for H^R , S^R , G^R , and V^R
2	PR and SRK parameterization workflows (a , b , $\alpha(T)$, mixing rules)
3	Stepwise integration procedures with Jacobian and chain-rule expansions

Applications

#	Application
1	Thermodynamic property estimation for phase equilibrium calculations (VLE, LLE)
2	Initialization and convergence aids in rigorous distillation and flash unit simulations
3	Development and validation of custom EOS-based property methods in process simulators

Related Concepts

#	Concept
1	Departure Functions
2	Cubic Equations of State
3	Thermodynamic Property Estimation

Tags

thermodynamics, equation-of-state, residual-properties