Formula 1

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Formula 2

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Formula 3

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Detailed Explanation

Equations of State are mathematical models that relate pressure (P), temperature (T), molar volume (V), and composition (z) for fluids—critical for predicting phase equilibria, enthalpy, entropy, fugacity, and transport properties in chemical, petroleum, and energy systems. Selecting the wrong EOS can lead to significant errors in process simulation (e.g., distillation column design, reservoir modeling, or refrigeration cycle analysis), especially near critical points, for polar or associating fluids, or under high-pressure conditions. The decision tree begins with fundamental fluid classification (e.g., nonpolar hydrocarbon vs. polar/associating vs. quantum fluid), then branches based on required fidelity (e.g., VLE-only vs. LLE + VLLE), operating range (subcritical to 100+ MPa), mixture complexity (binary to multicomponent with trace contaminants), and computational constraints (speed vs. thermodynamic consistency). It explicitly contrasts limitations: e.g., the ideal gas law fails above ~0.1 MPa for most organics; van der Waals lacks accurate acentric factor dependence; while PC-SAFT excels for polymers and hydrogen-bonding systems but demands extensive pure-component parameters and is computationally intensive. The poster integrates practical heuristics—such as 'use PR or SRK for sweet natural gas up to 20 MPa' or 'prefer CPA or ePCSAFT for water-containing systems'—and flags common pitfalls like using cubic EOS for supercritical CO? injection without volume translation correction.

Key Components

#	Component
1	Fluid Classification Matrix (nonpolar, polar, associating, quantum)
2	Condition-Based Branching Logic (P/T range, phase regime, accuracy requirement)
3	EOS Recommendation Grid with Strengths/Limitations Icons

Applications

#	Application
1	Process simulation in Aspen HYSYS or ChemCAD
2	Reservoir fluid modeling for enhanced oil recovery (EOR)
3	Design and safety analysis of high-pressure chemical reactors

Related Concepts

#	Concept
1	Fugacity coefficient
2	Phase equilibrium
3	Critical point prediction
4	Acentric factor
5	Thermodynamic consistency

Tags

> thermodynamics, equation-of-state, process-engineering, chemical-engineering, phase-equilibrium