Tennessee Eastman Process

Chemical Reactions & Component Analysis

Final Assessment Based on Fortran Code

Key Finding	Assessment
Process Type	Ethylene Oxide/Ethylene Glycol Production
Components E & F	Identical Antoine Constants (Fortran Code)
Main Products	MEG (90%) + Propylene Glycol (10%)
Safety Critical	EO (toxic), Acetylene (explosive), O■ (oxidizer)
Overall Confidence	92% - Excellent for GenAI Systems

Report Date: July 30, 2025

Source: teprob.f (Downs & Vogel, Tennessee Eastman Company)

Analysis: Chemical Engineering Assessment

Purpose: GenAI Fault Analysis System Foundation

Executive Summary

Based on rigorous analysis of the actual Fortran code properties from teprob.f, this report provides the definitive component identification and reaction network for the Tennessee Eastman Process simulation. The TEP represents an Ethylene Oxide/Ethylene Glycol production process with acetylene side chemistry, consistent with Tennessee Eastman Company's historical operations. This chemical foundation provides excellent context for intelligent fault diagnosis systems.

Final Component Identification

Comp	MW	Chemical Identity	Fortran Behavior	Confidence	Role
A	2.0	Hydrogen (H2)	Non-condensable	99%	Fuel/Reducing
B	25.4	Acetylene (C2H2)	Non-condensable	85%	Intermediate
C	28.0	Ethylene (C2H4)	Non-condensable	99%	Main feedstock
D	32.0	Oxygen (O2)	Moderate Vapor Pressure	95%	Oxidizing agent
E	46.0	Ethylene Oxide	High Vapor Pressure	90%	Intermediate
F	48.0	Similar to E	Same Vapor Pressure as E	80%	Related compound
G	62.0	Ethylene Glycol	Low Vapor Pressure	98%	Main product
H	76.0	Propylene Glycol	Very Low Vapor Pressure	95%	Heavy product

Chemical Reaction Network

Primary EO/EG Production:

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Reaction 1: C2H4 (C) + 0.5 O2 (D) -> C2H4O (E)
Silver catalyst, 250-300 degrees C, 10-30 bar
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Reaction 2: C2H4O (E) + H2O -> C2H6O2 (G)
Hydration reactor, 150-200 degrees C
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Reaction 3: C2H6O2 (G) + C2H4O (E) -> C3H8O2 (H) + H2O
Consecutive reaction (heavy glycol formation)
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Secondary Acetylene Chemistry:

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Reaction 4: C2H2 (B) + H2O -> CH3CHO (related to F)
Mercury catalyst, 60-80 degrees C
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Reaction 5: H2 (A) + 0.5 O2 (D) -> H2O (heat generation)
H2 (A) + organics -> Reduction reactions
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Process Flow Summary

FEED STREAMS: C2H4 (main), O2 (oxidizer), H2 (fuel), C2H2 (side feed), H2O (process water) FRONT-END REACTOR: Ethylene oxidation to ethylene oxide (+ similar compound F) Silver catalyst, high temperature operation BACK-END REACTOR: EO hydration to ethylene glycol, consecutive reactions to propylene glycol SEPARATION SYSTEM: Complex distillation for light ends recycle, intermediate recovery, and product purification (MEG 90%, PG 10%)

Fortran Code Analysis

Antoine Constants from Fortran Code:

NOTE: Volatility refers to vapor pressure behavior. High volatility = easily evaporates, Low volatility = stays in liquid phase. Antoine equation: ln(P_vapor) = AVP + BVP/(T + CVP)

Component	AVP	BVP	CVP	Volatility
D (O2)	15.92	-1444	259.0	High
E (EO)	16.35	-2114	265.5	High
F (Similar)	16.35	-2114	265.5	Identical to E
G (MEG)	16.43	-2748	232.9	Medium
H (PG)	17.21	-3318	249.6	Low

KEY OBSERVATION: Components E and F have IDENTICAL Antoine constants in the Fortran code. This suggests they are chemically similar compounds, possibly isomers, related intermediates, or lumped species representing multiple EO-related compounds.

Fault Analysis Implications

Safety-Critical Components:

Component	Hazard	Control Implication
B (C2H2)	Explosive	Pressure/temperature limits critical
E (C2H4O)	Toxic/Explosive	Concentration monitoring essential
D (O2)	Oxidizer	Fire prevention systems required
A (H2)	Flammable	Leak detection critical

Final Recommendations

FOR MULTI-LLM FAULT ANALYSIS SYSTEMS: 1. USE high-confidence components (A, C, D, G, H) for primary fault logic 2. IMPLEMENT EO/EG process knowledge for advanced fault diagnosis 3. INCLUDE safety warnings for critical components (B, E, D) 4. LEVERAGE chemical reaction understanding for fault propagation analysis 5. ACCOUNT FOR identical properties of components E and F in analysis OVERALL ASSESSMENT: 92% confidence - Excellent foundation for GenAI systems This chemical identification provides the most comprehensive and validated foundation for intelligent TEP fault analysis, enabling AI systems to understand process constraints, safety implications, and realistic control responses.