Relatório de Validação DWSIM

Suíte de Testes Automatizados - Fluent API

03/05/2026

TODAS AS 316 VERIFICAÇÕES PASSARAM

72 casos de teste | 316 verificações | 8 categorias

Resumo por Categoria

Categoria	Testes	Verif.	Aprovadas	Reprov.	Status
Termodinâmica	18	30	30	0	**PASS**
Operações Unitárias - Básicas	8	22	22	0	**PASS**
Operações Unitárias - Avançadas	5	19	19	0	**PASS**
Bioprocessos	10	44	44	0	**PASS**
Compostos	2	11	11	0	**PASS**
Refino (Plus)	6	37	37	0	**PASS**
Configuração de Pacotes Termodinâmicos	2	6	6	0	**PASS**
Fluxogramas de Processo Completos	20	146	146	0	**PASS**
TOTAL	**71**	**315**	**315**	**0**	**PASS**

Termodinâmica

T02 - Steam Tables - water T_sat @ 1 atm

PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_sat (NIST 373.124 K)	373.124	373.1243	0.00	0.50	K	PASS

T03 - NRTL - ethanol/water azeotrope @ 1 atm, z_EtOH = 0.894

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_az (Gmehling 351.45 K)	351.45	351.541327	+0.03	1.00	K	PASS
y_EtOH ≈ x_EtOH	0.895686	0.892314	-0.38	2.00	-	PASS

T04 - PR EOS - CH4 @ 500 K, 1 bar (ideal gas limit)

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ vs ideal gas (PM/RT)	0.385855	0.385945	+0.02	0.50	kg/m^3	PASS
Vapor fraction (expected =1)	1	1	0.00	0.10	-	PASS

T05 - SRK - propane P_sat @ 298.15 K (NIST 9.49 bar)

PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
P_sat	949000	9.6e+05	+1.16	5.00	Pa	PASS

T06 - PR78 - liquid n-heptane @ 25 °C, 1 atm

PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ_liq (NIST 679.5)	679.5	681.043168	+0.23	5.00	kg/m^3	PASS

T07 - LKP - CH4 gas @ 300 K, 1 bar (Z≈1)

PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ vs ideal gas	0.643092	0.644254	+0.18	1.00	kg/m^3	PASS

T08 - UNIQUAC - EtOH/H2O azeotrope @ 1 atm

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_az (Gmehling 351.45 K)	351.45	351.486203	+0.01	2.00	K	PASS
y_EtOH ≈ x_EtOH	0.896328	0.891672	-0.52	5.00	-	PASS

T09 - Wilson - equimolar MeOH/H2O @ 1 atm, bubble point — PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_bubble between pure b.p.	[337.7,373.1	346.055593	-	-	K	PASS
y_MeOH > x_MeOH (more volatile)	[0.5,1]	0.781689	-	-	-	PASS

T10 - UNIFAC (predictive) - EtOH/H2O @ 1 atm — PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_az (351.45 K, tol 3%)	351.45	351.506737	+0.02	3.00	K	PASS
y_EtOH ≈ x_EtOH	0.894696	0.893304	-0.16	10.00	-	PASS

T11 - Mod UNIFAC (Dortmund) - equimolar Acetone/H2O @ 1 atm — PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_bubble between pure b.p.	[329.2,373.1	332.775356	-	-	K	PASS
y_Acetone > x_Acetone	[0.5,1]	0.841821	-	-	-	PASS

T12 - Raoult - equimolar Benzene/Toluene @ 1 atm — PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_bubble (Smith VN ≈ 365 K)	365	365.359189	+0.10	2.00	K	PASS
y_Benzene (≈ 0.71)	0.71	0.714146	+0.58	5.00	-	PASS

T13 - Seawater (IAPWS-08) - S=35 g/kg, 25 °C, 1 atm — PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ (IAPWS-08 ≈ 1023.4)	1023.4	1024.174155	+0.08	1.00	kg/m^3	PASS

T14 - PRSV2-M - methanol P_sat @ 337.7 K (b.p. ≈ 1 atm) — PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
P_sat	101325	1.011e+05	-0.21	5.00	Pa	PASS

T15 - Grayson-Streed - C3/C4 50/50 @ 300 K, 5 bar — PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Vapor frac in (0,1) - two phases	[0.01,0.99]	0.433573	-	-	-	PASS
x_C4 > 0.5 (heavy liquid)	[0.5,1]	0.624643	-	-	-	PASS
y_C3 > 0.5 (light vapor)	[0.5,1]	0.662842	-	-	-	PASS

T16 - UNIFAC-LL - H2O/n-hexane 50/50 @ 25 °C (smoke) PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T preserved	298.15	298.15	0.00	0.10	K	PASS
Mass enthalpy finite	[-1000000,10	-699.000545	-	-	kJ/kg	PASS

T17 - PR vs SRK - natural gas (90/7/3) @ 250 K, 50 bar PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ_SRK $\approx$ ρ_PR ($\pm$ 5 %)	56.162689	55.072427	-1.94	5.00	kg/m^3	PASS
ρ_PR > 0	[1,1000]	56.162689	-	-	kg/m^3	PASS

T18 - Chao-Seader - C3/n-C4 50/50 @ 320 K, 8 bar PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Vapor frac in (0,1)	[0.01,0.99]	0.530372	-	-	-	PASS
y_C3 > 0.5 (more volatile)	[0.5,1]	0.617442	-	-	-	PASS

T19 - Mod UNIFAC (NIST) - toluene P_sat @ 383.78 K (b.p. $\approx$ 1 atm) PASS[1/1]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
P_sat	101325	102033.48452	+0.70	5.00	Pa	PASS

Operações Unitárias - Básicas

U01 - Heater - H2O 1 kg/s, 25 80 °C

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_out	353.15	353.149995	0.00	0.10	K	PASS
Heat duty (NIST 230±5 kW)	[225,235]	230.062304	-	-	kW	PASS

U02 - Cooler - H2O 1 kg/s, 80 25 °C

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_out	298.15	298.150002	0.00	0.10	K	PASS
Heat removed (NIST 230±5 kW)	[225,235]	230.062304	-	-	kW	PASS

U03 - Pump - H2O 1 kg/s, ΔP=10 bar, η=75 %

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ΔP	1000000	1000000	0.00	0.10	Pa	PASS
Power (V·ΔP/η)	1.337345	1.337281	0.00	5.00	kW	PASS

U04 - Counter-current HX - H2O 1 kg/s @ 100 ? vs 25 ?

PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
q_hot vs Q	218.510917	218.510917	0.00	1.00	kW	PASS
q_cold vs Q	218.510917	218.510915	0.00	1.00	kW	PASS
Balance (q_hot - q_cold)/Q	0	0	0.00	1.00	-	PASS
Q > 0 (transfer occurred)	[1,1000000]	218.510917	-	-	kW	PASS

U05 - Isentropic compressor - N2 1 5 bar, T_in=300 K

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_out (γ=1.4 ideal ≈ 475 K)	475.145883	474.136858	-0.21	3.00	K	PASS
P_out	[499000,5010	500000	-	-	Pa	PASS
Work > 0	[0.1,1000000	5.09507	-	-	kW	PASS

U06 - Isentropic expander - N2 10 1 bar, T_in=500 K

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_out (γ=1.4 ideal ≈ 259 K)	258.973734	259.637621	+0.26	3.00	K	PASS
Generated work > 0	[0.1,1000000	7.031766	-	-	kW	PASS

U07 - Isenthalpic valve - CO2 100 10 bar, T_in=300 K (JT effect) PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
h_in ≈ h_out	-238.370028	-238.370028	0.00	0.10	kJ/kg	PASS
T_out < T_in (μ_JT > 0)	[200,299.99]	232.933896	-	-	K	PASS
P_out	[999000,1001	1000000	-	-	Pa	PASS

U08 - Splitter - H2O 100 kg/s, ratio 70/30 PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
m_out1	70	70	0.00	0.10	kg/s	PASS
m_out2	30	30	0.00	0.10	kg/s	PASS
T_out1 = T_in	350	350	0.00	0.10	K	PASS
T_out2 = T_in	350	350	0.00	0.10	K	PASS

Operações Unitárias - Avançadas

A01 - EtOH/H2O distillation - NRTL, 20 stages, RR=2, B=75 mol/s

PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Global balance F = D + B	100	100	0.00	0.10	mol/s	PASS
B (specified)	75	75	0.00	0.10	mol/s	PASS
Distillate rich in EtOH (>50%)	[0.5,1]	0.808752	-	-	-	PASS
Bottoms lean in EtOH (<50%)	[0,0.5]	0.397083	-	-	-	PASS
Condenser duty > 0	[0,100000000	2927.543634	-	-	kW	PASS
Reboiler duty > 0	[0,100000000	3608.806278	-	-	kW	PASS

A02 - Conv Reactor - CH4+2H2O CO2+4H2 at 50% (stoichiometry)

PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
CH4 out	1	1	0.00	0.50	mol/s	PASS
H2O out	4	4	0.00	0.50	mol/s	PASS
CO2 out	1	1	0.00	0.50	mol/s	PASS
H2 out	4	4	0.00	0.50	mol/s	PASS

A03 - Eq Reactor - WGS @ 1100 K, Keq=1 (ln(K)=0)

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Q ≈ Keq = 1.0	1	1.006865	+0.69	5.00	-	PASS
C balance (CO_in - CO_out = CO2_out)	0.500855	0.500855	0.00	0.50	mol/s	PASS
H balance (H2O reacted = H2 formed)	0.500855	0.500855	0.00	0.50	mol/s	PASS

A04 - Adiabatic mixer - H2O 100 kg/s@300K + 50 kg/s@348K

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Mass balance m1+m2=m3	150	150	0.00	0.01	kg/s	PASS
Energy balance ΣmH_in=ΣmH_out	26936.276376	26936.276354	0.00	0.10	kW	PASS
T_out within [300, 348] K	[300,348]	316.010042	-	-	K	PASS

A05 - Gibbs Reactor - steam reforming CH4 @ 1100 K, 1 bar

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
CH4 conversion > 95 %	[0.95,1]	0.998722	-	-	-	PASS
H2 produced > 2 mol/s	[2,4]	3.323805	-	-	mol/s	PASS
(CO + CO2) ≈ CH4 reacted	[0.95,1.05]	1	-	-	-	PASS

Bioprocessos

B01 - BioReactor Monod - continuous alcoholic fermentation

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Total outlet mass finite	[0.1,100]	2.967976	-	-	kg/s	PASS
Glucose consumed (>0)	[0.001,0.1]	0.034883	-	-	kg/s	PASS
Ethanol produced > 0	[0,1]	0.078417	-	-	kg/s	PASS

B02 - Anaerobic Digester Black-Box - glucose, HRT 20 d

PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Total mass finite	[0.5,5]	1.165324	-	-	kg/s	PASS
Glucose removed > 50 %	[0.025,0.05]	0.04	-	-	kg/s	PASS
CH4 produced > 0	[0,1]	0.041319	-	-	kg/s	PASS
CH4 mass fraction in biogas > 20 %	[0.2,1]	0.26717	-	-	-	PASS

B03 - Centrifuge - DiskStack solve, 10 kg/s

PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Mass balance F = H + L	10	10	0.00	0.10	kg/s	PASS
FeedMass result	10	10	0.00	0.10	kg/s	PASS
HeavyMass result	0.935	0.935	0.00	0.10	kg/s	PASS
Heavy enriched in biomass (>40 %)	[0.4,1]	0.508021	-	-	-	PASS
Light enriched in water (>90 %)	[0.9,1]	0.943188	-	-	-	PASS

B04 - Chromatography Bind&Elute - IEX, ethanol capture

PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Feed mass	1	1	0.00	0.10	kg/s	PASS
Balance F = P + W	1	1	0.00	0.10	kg/s	PASS
Ethanol in product ≈ 0.095 kg/s (95 % recovery)	[0.09,0.1]	0.095	-	-	kg/s	PASS

B05 - Cell Lysis HPH - E. coli, 80 MPa × 2 passes

PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Feed mass	1	1	0.00	0.10	kg/s	PASS
Balance F = L + D	1	1	0.00	0.10	kg/s	PASS
Lysate > debris (mass)	[1,100000000	8.756098	-	-	-	PASS
Ethanol majority in lysate	[0.04,0.05]	0.0475	-	-	kg/s	PASS

B06 - Crossflow UF - Concentration VCF=10 PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Feed mass	10	10	0.00	0.10	kg/s	PASS
Mass balance F = R + P	10	10	0.00	0.10	kg/s	PASS
Effective VCF ≈ 10	[9,11]	10	-	-	-	PASS
Ethanol in retentate > 90 %	[0.09,0.1]	0.1	-	-	kg/s	PASS
Permeate nearly pure water	[0.95,1]	0.979798	-	-	-	PASS

B07 - Cooling Crystallizer - Glucose/H2O 0.6/0.4 kg/s, 80 5 °C PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Solute in feed	0.6	0.6	0.00	0.10	kg/s	PASS
Csat(5 °C) between 0.2 and 0.5 g/g	[0.2,0.5]	0.3	-	-	g/g	PASS
Yield > 50 % (wide cooling)	[0.5,1]	0.8	-	-	-	PASS
Crystals > 0	[0,1]	0.48	-	-	kg/s	PASS
Mass balance	1	1	0.00	0.10	kg/s	PASS

B08 - Biogas Upgrader Amine - biogas biomethane PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Feed mass	1	1	0.00	0.10	kg/s	PASS
Mass balance	1	1	0.00	0.10	kg/s	PASS
Biomethane CH4 purity > 90 %	[0.9,1]	0.958517	-	-	-	PASS
CH4 recovery > 99 %	[0.99,1]	0.999	-	-	-	PASS
Wobbe Index > 0	[1,1000000]	34.410752	-	-	-	PASS

B09 - Pretreatment DiluteAcid - log R0=3.6 PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Severity R0 = 10^logR0	3981.07	3981.071706	0.00	0.10	-	PASS
Mass balance F = slurry	1	1	0.00	0.10	kg/s	PASS
T_out preserved	303.15	303.15	0.00	0.10	K	PASS
Glucose preserved (no cellulose role)	[0.179,0.181	0.18	-	-	kg/s	PASS

B10 - CFB Fast Pyrolysis - pine, T_sand=833 K PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Yields sum ≈ 1	[0.95,1.05]	1	-	-	-	PASS
Oil yield > 0	[0.001,1]	0.692121	-	-	-	PASS
Gas yield > 0	[0.001,1]	0.017254	-	-	-	PASS
Char yield > 0	[0.001,1]	0.014963	-	-	-	PASS
T_out within pyrolysis range (700-820 K)	[700,820]	774.038879	-	-	K	PASS
Pyrolysis duty > 0 (endothermic)	[1,1000000]	250	-	-	kW	PASS

Compostos

C01 - Pseudocomponent - Cut_650K (NBP=650 K, SG=0.85, MW=240) PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
NBP preserved	650	650	0.00	0.00	K	PASS
MW preserved	240	240	0.00	0.00	g/mol	PASS
Tc > NBP (Riazi-Daubert)	[650,1200]	818.075924	-	-	K	PASS
Pc within 5-50 bar	[500000,5000	1.148e+06	-	-	Pa	PASS
Acentric factor > 0	[0.05,1.5]	0.794626	-	-	-	PASS
Watson K within paraffinic range (10-13)	[10,13]	12.396803	-	-	-	PASS
Density computed @ 700 K	[1,100]	4.393518	-	-	kg/m^3	PASS

C02 - Compound from JSON - Biomass_Yeast.json PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Compound registered	[1,1]	1	-	-		PASS
MW loaded	2478.45	2478.45	0.00	0.10	g/mol	PASS
OriginalDB = User	[1,1]	1	-	-		PASS
Has C element	[1,1]	1	-	-		PASS

Refino (Plus)

R01 - HDS - hydrodesulfurization

PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Reactor T	623.15	623.15	0.00	0.00	K	PASS
Reactor P	4000000	4000000	0.00	0.00	Pa	PASS
LHSV	2	2	0.00	0.00	h^{-1}	PASS
PreExponential k0	150000000	150000000	0.00	0.10		PASS
Activation Energy	110000	110000	0.00	0.00	J/mol	PASS
EnableHDN = true	[1,1]	1	-	-		PASS
Mercaptan conv	0.99	0.99	0.00	0.00	-	PASS

R02 - Reformer - RON 95 100

PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Reactor T	793.15	793.15	0.00	0.00	K	PASS
Reactor P	1500000	1500000	0.00	0.00	Pa	PASS
Base RON	95	95	0.00	0.00	-	PASS
Target RON	100	100	0.00	0.00	-	PASS
Base reformate	0.83	0.83	0.00	0.00	-	PASS
H2 sensitivity / RON	0.0015	0.0015	0.00	0.00	-	PASS

R03 - FCC - slate yields, conv 78 %

PASS[8/8]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
YieldMethod = Slate	[0,0]	0	-	-		PASS
Reactor T	773.15	773.15	0.00	0.00	K	PASS
Reactor P	250000	250000	0.00	0.00	Pa	PASS
C/O ratio	7	7	0.00	0.00	-	PASS
Target conv	0.78	0.78	0.00	0.00	-	PASS
Base gasoline yield	0.46	0.46	0.00	0.00	-	PASS
Base LPG yield	0.18	0.18	0.00	0.00	-	PASS
Base coke yield	0.04	0.04	0.00	0.00	-	PASS

R04 - Hydrocracker - conv 65 %, P=150 bar

PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Reactor T	673.15	673.15	0.00	0.00	K	PASS
Reactor P	15000000	15000000	0.00	0.00	Pa	PASS
LHSV	1	1	0.00	0.00	h^{-1}	PASS
Target conversion	0.65	0.65	0.00	0.00	-	PASS
H2 consumption	0.025	0.025	0.00	0.00	kg/kg	PASS
S removal	0.99	0.99	0.00	0.00	-	PASS
N removal	0.95	0.95	0.00	0.00	-	PASS

R05 - Coker - heater 500 °C, drum 2 bar

PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Heater outlet T	773.15	773.15	0.00	0.00	K	PASS
Drum P	200000	200000	0.00	0.00	Pa	PASS
Heater duty / kg feed	450000	450000	0.00	0.00	J/kg	PASS
Coke / CCR factor	1.6	1.6	0.00	0.00	-	PASS
Dry gas / total gas	0.25	0.25	0.00	0.00	-	PASS
LGO / gas oil	0.55	0.55	0.00	0.00	-	PASS
UseFeedPNA = true	[1,1]	1	-	-		PASS

R06 - Blender - 3 inlets, P-mode Min

PASS[2/2]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
NumberOfInlets	3	3	0.00	0.00	-	PASS
PressureMode = Min	[1,1]	1	-	-		PASS

Configuração de Pacotes Termodinâmicos

P01 - PR - kij effect on CO2/N2 (300 K, 100 bar) PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
ρ with kij=0 finite	[1,1000]	178.379111	-	-	kg/m^3	PASS
ρ with kij=0.4 finite	[1,1000]	164.815776	-	-	kg/m^3	PASS
Difference $\lvert\rho$(kij=0.4) - ρ(kij=0)$\rvert$ > 0.5 kg/m^3	[0.5,1000000	13.563335	-	-	kg/m^3	PASS

P02 - NRTL - effect of EtOH/H2O BIPs on bubble point @ 1 atm, x=0.5 PASS[3/3]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
T_bubble with default-like BIPs > 350 K	[350,380]	355.96038	-	-	K	PASS
T_bubble with strong BIPs finite	[300,400]	338.79259	-	-	K	PASS
Δ T_bubble > 0.1 K (BIPs altered the flash)	[0.1,50]	17.16779	-	-	K	PASS

Fluxogramas de Processo Completos

F01 - F01 - Refrigeration cycle (propane, R-290) PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Compressor work > 0	[0.001,100]	4.20275	-	-	kW	PASS
Condenser heat > 0 (rejection)	[0.001,100]	15.93719	-	-	kW	PASS
Evaporator heat > 0 (absorption)	[0.001,100]	11.734806	-	-	kW	PASS
Balance Q_cond ≈ Q_evap + W_comp	15.937557	15.93719	0.00	0.50	kW	PASS
Cycle closure: T_5 ≈ T_1	252.99458	253	0.00	0.50	K	PASS
Refrigeration COP within 2-7	[2,7]	2.792173	-	-	-	PASS

F02 - F02 - Mini ethanol plant (Gay-Lussac fermentation 95 %) PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Reactor balance F = liq + gas	10	10	0.00	0.50	kg/s	PASS
Post-cooler preserves mass	9.527684	9.527684	0.00	0.10	kg/s	PASS
CO2 leaves with gas phase (>50 %)	[0.5,1]	0.959111	-	-	-	PASS
Ethanol in final broth (3-7 %)	[0.03,0.08]	0.050109	-	-	-	PASS
Low residual glucose (<2 %)	[0,0.02]	0.005248	-	-	-	PASS
Post-cooler T_out = 25 °C	298.15	298.15	0.00	0.10	K	PASS

F03 - F03 - Natural gas processing PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Global balance: feed = gas + NGL + water	1.760511	1.760511	0.00	0.50	kg/s	PASS
Dry gas enriched in CH4 (>85 %)	[0.85,1]	0.909049	-	-	-	PASS
Residual water in gas < 1 %	[0,0.01]	0.000046	-	-	-	PASS
Condensed liquids (NGL + water) > 0	[0,10]	0.017933	-	-	kg/s	PASS
Export compressor work > 0	[0.001,10000	113.736875	-	-	kW	PASS
P_export = 80 bar	[7990000,801	8000000	-	-	Pa	PASS

F04 - F04 - Ammonia synthesis (single-pass) PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
N2 conversion within 5-99 %	[0.05,0.99]	0.487898	-	-	-	PASS
H atomic balance	6	6	0.00	0.50	mol/s	PASS
N atomic balance	2	2	0.00	0.50	mol/s	PASS
NH3 produced > 0	[0,2]	0.975797	-	-	mol/s	PASS
Liquid enriched in NH3 (>50 %)	[0.5,1]	0.990677	-	-	-	PASS
Purge gas predominantly H2/N2	[0,0.5]	0.021813	-	-	-	PASS

F05 - F05 - Mini refinery (Plus): config applied — PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
HDS LHSV	2	2	0.00	0.00	h^{-1}	PASS
Reformer target RON	100	100	0.00	0.00	-	PASS
FCC base gasoline	0.46	0.46	0.00	0.00	-	PASS
Blender N inlets	3	3	0.00	0.00	-	PASS
Pseudo component MW	110	110	0.00	0.00	g/mol	PASS
Pseudo Tc computed > NBP	[420,800]	599.456689	-	-	K	PASS

F06 - F06 - 2G fermentation train — PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Pretreatment passes mass (>0)	[1,100]	10.325579	-	-	kg/s	PASS
BioReactor produces ethanol	[0,10]	0.792548	-	-	kg/s	PASS
Centrifuge balance F = H + L	22.885548	22.885548	0.00	0.50	kg/s	PASS
Cream enriched in biomass (>10 %)	[0.1,1]	0.164977	-	-	-	PASS
Ethanol predominant in clarified broth	[0.005,0.1]	0.034972	-	-	-	PASS

F07 - F07 - Full DSP (Lysis Centrifuge Chromatography) — PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Lysis balance F = lysate + debris	1	1	0.00	0.50	kg/s	PASS
Centrifuge balance F = cake + clarified	0.8975	0.8975	0.00	0.50	kg/s	PASS
Chromatography balance F = prod + waste	0.852625	0.852625	0.00	0.50	kg/s	PASS
Product > 0 at each step	[0,1]	0.0095	-	-	kg/s	PASS
Product retained after centrifuge	[0,1]	0.009025	-	-	kg/s	PASS
Overall product recovery > 70 %	[0.7,1]	0.8303	-	-	-	PASS

F08 - F08 - WWTP biogas grid biomethane — PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
AD produces biogas (>0)	[0,1]	0.284358	-	-	kg/s	PASS
Biomethane generated (>0)	[0,1]	0.077981	-	-	kg/s	PASS
Biomethane rich in CH4 (>85 %)	[0.85,1]	0.973277	-	-	-	PASS
Residual CO2 in biomethane < 5 %	[0,0.05]	0.026723	-	-	-	PASS
Compressor delivers 50 bar	[4990000,501	5000000	-	-	Pa	PASS
Compressor work > 0	[0.001,10000	90.330919	-	-	kW	PASS

F09 - F09 - Microalgae cultivation (PBR + UF + Crystallizer) PASS[6/6]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Bioreactor produces broth (>0)	[0.1,10]	2.119076	-	-	kg/s	PASS
UF balance: F = retentate + permeate	2.119076	2.119076	0.00	0.50	kg/s	PASS
Crystallizer balance: F = crystals + liquor	0.22277	0.22277	0.00	0.50	kg/s	PASS
Concentrate enriched in biomass	[0.005,1]	0.054177	-	-	-	PASS
Permeate nearly free of biomass	[0,0.005]	0	-	-	-	PASS
Solid crystals >= 0	[0,10]	0	-	-	kg/s	PASS

F10 - F10 - Green hydrogen (solar + electrolysis) PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Solar power > 0	[1,1000]	200	-	-	kW	PASS
H2 in H2-rich stream	[0.5,1]	0.993653	-	-	-	PASS
O2 in O2-rich stream	[0.001,1]	0.173011	-	-	-	PASS
H2 product mass > 0	[0.001,100]	0.398805	-	-	kg/s	PASS
O2 product mass > 0	[0.001,100]	2.6555	-	-	kg/s	PASS

F11 - F11 - Bz/Tol distillation with feed preheat PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Molar balance F = D + B	100	100	0.00	0.10	mol/s	PASS
Bottoms flow B = 50	50	50	0.00	0.10	mol/s	PASS
Distillate rich in Bz (>85%)	[0.85,1]	0.999904	-	-	-	PASS
Bottoms rich in Tol (>85%)	[0.85,1]	0.999795	-	-	-	PASS
Feed preheated above 300 K	[300.1,400]	331.455166	-	-	K	PASS
Condenser duty > 0	[0,100000000	6298.848132	-	-	kW	PASS
Reboiler duty > 0	[0,100000000	6881.043918	-	-	kW	PASS

F12 - F12 - Sour gas sweetening (Amine + Claus) PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Sweet gas H2S < 1%	[0,0.01]	0.000393	-	-	-	PASS
CH4 retention > 90%	[0.9,1.01]	0.99	-	-	-	PASS
AT mass balance	14.015639	14.015639	0.00	1.00	kg/s	PASS
Claus produces sulfur > 0	[0,10]	1.576132	-	-	kg/s	PASS
Claus produces tail gas > 0	[0,10]	1.080482	-	-	kg/s	PASS

F13 - F13 - VGO hydrocracking (Plus) PASS[5/5]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Mixed feed mass > 0	[10,100]	24.31966	-	-	kg/s	PASS
Mixer mass balance	24.31966	24.31966	0.00	1.00	kg/s	PASS
HCR conversion config	0.7	0.7	0.00	0.00	-	PASS
HCR LHSV config	1	1	0.00	0.00	h^{-1}	PASS
HCR ran (partial)	[1,1]	1	-	-	-	PASS

F14 - F14 - Reverse osmosis desalination (Plus) PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Pump outlet ~60 bar	[5990000,601	6000000	-	-	Pa	PASS
Permeate EtOH lower than feed	[0,0.035]	0.035	-	-	-	PASS
Recovery ratio > 0	[0.001,0.95]	0.0198	-	-	-	PASS
RO mass balance	10	10	0.00	1.00	kg/s	PASS

F15 - F15 - Methanol synthesis from syngas PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
CO conversion 20-99%	[0.2,0.99]	0.692412	-	-	-	PASS
C atomic balance across reactor	1.5	1.499999	0.00	1.00	mol/s	PASS
Separator balance	0.058078	0.058078	0.00	0.50	kg/s	PASS
Compressor work > 0	[0.001,10000	34.98396	-	-	kW	PASS

F16 - F16 - Hydroelectric turbine + heat recovery PASS[4/4]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
Turbine power 10-40 kW	[10,40]	20.825	-	-	kW	PASS
Hot side cools (< 353 K)	[280,352]	320.488902	-	-	K	PASS
Cold side warms (> 288 K)	[289,360]	291.316205	-	-	K	PASS
Cold side mass conservation	50	50	0.00	1.00	kg/s	PASS

F17 - F17 - Naphtha HDS + Isomerization (Plus) PASS[7/7]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
HDS removes H2S (< 1%)	[0,0.01]	0.006578	-	-	-	PASS
Isomerate produced > 0	[0.1,50]	12.849285	-	-	kg/s	PASS
HDS LHSV config	3	3	0.00	0.00	h^{-1}	PASS
ISO RON config	82	82	0.00	0.00	-	PASS
ISO yield config	0.9	0.9	0.00	0.00	-	PASS
HDS mass balance	15.202263	15.202263	0.00	5.00	kg/s	PASS
ISO mass balance	15.202263	15.202263	0.00	5.00	kg/s	PASS

F18 - F18 - Anaerobic digester: BlackBox + ADM1-Lite + ADM1-Full

PASS[17/17]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
[BB] COD removal ~80%	[0.5,0.95]	0.8	-	-	-	PASS
[BB] CH4 mole frac ~65%	[0.4,0.9]	0.65	-	-	-	PASS
[BB] Specific CH4 yield > 0	[0,1]	0.000202	-	-	Nm^3/kgCOD	PASS
[BB] Effluent mass > 0	[0.1,10]	1.010671	-	-	kg/s	PASS
[BB] Biogas mass > 0	[0,1]	0.154653	-	-	kg/s	PASS
[ADM1L] COD removal > 0	[0.001,1]	0.999999	-	-	-	PASS
[ADM1L] CH4 yield > 0	[0,2]	0.314625	-	-	Nm^3/kgCOD	PASS
[ADM1L] Acetogen pop > 0 [0,100]	2.073736	-	-	g	VSS/L	PASS
[ADM1L] Methanogen pop > 0 [0,100]	2.660775	-	-	g	VSS/L	PASS
[ADM1L] Effluent mass > 0	[0.1,10]	1.00552	-	-	kg/s	PASS
[ADM1L] Biogas mass > 0	[0,1]	0.214214	-	-	kg/s	PASS
[ADM1F] COD removal > 0	[0.001,1]	0.703379	-	-	-	PASS
[ADM1F] CH4 yield > 0	[0,2]	0.377019	-	-	Nm^3/kgCOD	PASS
[ADM1F] Effluent mass > 0	[0.1,10]	1.011086	-	-	kg/s	PASS
[ADM1F] Biogas mass > 0	[0,1]	0.186902	-	-	kg/s	PASS
[ADM1F] Profile series count > 0	[1,50]	36	-	-	-	PASS
[ADM1F] Profile DataTable rows > 0	[1,1000000]	10	-	-	rows	PASS

F19 - F19 - BioReactor: 3 modes × 3 kinetics + profiles

PASS[17/17]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
[A] Continuous mass > 0	[0.1,10]	3.05572	-	-	kg/s	PASS
[A] Glucose consumed	[0.001,0.11]	0.11	-	-	kg/s	PASS
[A] Ethanol produced	[0,1]	0.06607	-	-	kg/s	PASS
[A] Profile series count > 0	[1,20]	9	-	-	-	PASS
[A] Profile CSV length > 0	[10,10000000	44849	-	-	chars	PASS
[A] Profile DataTable rows > 0	[1,1000000]	502	-	-	rows	PASS
[B] Batch mass > 0	[0.1,10]	2.04538	-	-	kg/s	PASS
[B] Glucose consumed (Haldane)	[0.001,0.3]	0.001571	-	-	kg/s	PASS
[B] Ethanol produced (Haldane)	[0,1]	0.01667	-	-	kg/s	PASS
[B] Outlet T >= feed (adiabatic)	[303,500]	303.15	-	-	K	PASS
[B] Profile S series points > 10	[10,1000000]	501	-	-	pts	PASS
[B] Profile S[0] > 0	[1,10000000]	2.926e+05	-	-	-	PASS
[C] FedBatch mass > 0	[0.1,10]	2.028321	-	-	kg/s	PASS
[C] Glucose consumed (Contois)	[0.001,0.05]	0.05	-	-	kg/s	PASS
[C] Ethanol produced (Contois)	[0,1]	0.03036	-	-	kg/s	PASS
[C] Profile X final > 0	[1,100000000	15273.412738	-	-	-	PASS
[C] Profile X points > 10	[10,1000000]	501	-	-	pts	PASS

F20 - F20 - CFB fast pyrolysis: 2 feedstocks × 2 sand modes — PASS[18/18]

Verificação	Esperado	Calculado	Err %	Tol %	Unid.	
[A] Pine yields ≈ 1	[0.95,1.05]	1	-	-	-	PASS
[A] Bio-oil yield > 0	[0.01,0.95]	0.803581	-	-	-	PASS
[A] Gas yield > 0	[0.005,0.5]	0.0246	-	-	-	PASS
[A] Char yield > 0	[0.005,0.5]	0.021338	-	-	-	PASS
[A] T_out 650-850 K	[650,850]	793.617988	-	-	K	PASS
[A] Vapor residence < 3 s	[0.01,3]	0.94305	-	-	s	PASS
[A] Pyrolysis duty > 0	[1,1000000]	250	-	-	kW	PASS
[A] Profile series count > 0	[1,50]	14	-	-	-	PASS
[A] Profile T_K points > 0	[2,1000]	41	-	-	pts	PASS
[A] Profile CSV length > 0	[10,10000000	7770	-	-	chars	PASS
[B] Residue yields ≈ 1	[0.95,1.05]	1	-	-	-	PASS
[B] Bio-oil yield > 0	[0.01,0.95]	0.739817	-	-	-	PASS
[B] Gas yield > 0	[0.005,0.5]	0.011349	-	-	-	PASS
[B] Char yield > 0	[0.005,0.5]	0.008983	-	-	-	PASS
[B] T_out 600-900 K	[600,900]	726.719382	-	-	K	PASS
[B] Combustor duty > 0	[1,1000000]	261.406212	-	-	kW	PASS
[B] Sand circulation > 0	[0.1,100]	7.590498	-	-	kg/s	PASS
[B] Profile DataTable rows > 0	[2,1000]	51	-	-	rows	PASS