Furnace Carbon Activity and Carbon Potential from CO and CO_2

Carbon activity of a furnace atmosphere from CO and CO_2 partial pressures via the Boudouard equilibrium, and the equivalent carbon content in austenite.

Method: Boudouard equilibrium with 298 K standard data; NIST Chemistry WebBook; ...

Input parameters

Unit system: SI

Parameter	Value	Unit
CO partial pressure	20.000	kPa
CO_2 partial pressure	0.15000	kPa
Furnace temperature	925.00	°C
Reaction enthalpy (C + CO_2 → 2CO)	172.45	kJ/mol
Reaction entropy (J/(mol·K))	175.79	
Carbon in austenite at graphite saturation	1.2500	%

Calculated results

Parameter	Value	Unit
Standard free energy	-38.173	kJ/mol
Equilibrium constant	46.148	
Carbon activity	0.57785	
Carbon potential (approximate)	0.72232	%

Notes for this case

• C + CO_2 ⍰ 2CO: K = (p_CO/p°)²/[a_C(p_CO_2/p°)], so a_C = p_CO²/(K·p_CO_2·p°). ΔG° = ΔH° − TΔS° uses 298 K standard data (Ellingham approximation, editable). Carbon potential ≈ a_C·C_sat assumes Henrian behaviour of carbon in austenite; real atmospheres are controlled from dew point or O_2 probes calibrated against shim stock. a_C above 1 means sooting.

Formula and method

$$a_C = \frac{(p_{CO}/p^\circ)^2}{K\,(p_{CO_2}/p^\circ)}, \quad K = e^{-\Delta G^\circ/RT}, \quad \Delta G^\circ = \Delta H^\circ - T\Delta S^\circ, \quad C_p \approx a_C C_{sat}$$

Variables

p_{CO}	CO partial pressure	Pa
p_{CO_2}	CO_2 partial pressure	Pa
T	Furnace temperature	K
ΔH°	Reaction enthalpy (C + CO_2 → 2CO)	J/mol
ΔS°	Reaction entropy (J/(mol·K))	-
C_{sat}	Carbon in austenite at graphite saturation	-
ΔG°	Standard free energy	J/mol
K	Equilibrium constant	-
a_C	Carbon activity	-
C_p	Carbon potential (approximate)	-

Method and standards

Carbon potential.

Assumptions and limits

- Ideal gases; Ellingham approximation; Henrian carbon in austenite.

References

Boudouard equilibrium with 298 K standard data, NIST Chemistry WebBook, standard enthalpies of formation and entropies (CO, CO_2, graphite)

Report details

Report reference	FCC-YERZ-SGTK (the same inputs always give the same reference)
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Release checks	3 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/materials/heat-treatment/carbon-potential-co-co2

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.