Water-Gas Shift Equilibrium Conversion

Equilibrium constant of the water-gas shift reaction at a temperature and the equilibrium CO conversion and exit composition from a feed of CO, H2O, CO2 and H2.

Method: Water-gas shift equilibrium

Input parameters

Unit system: SI

Parameter	Value	Unit
Reactor exit temperature	350.00	°C
CO in feed (mol)	10.000	
Steam in feed (mol)	30.000	
CO_2 in feed (mol)	5.0000	
H_2 in feed (mol)	45.000	

Calculated results

Parameter	Value	Unit
Equilibrium constant	20.414	
Equilibrium CO conversion	83.814	%
Extent of reaction (mol)	8.3814	
CO in the dry exit gas	2.3670	%
H_2 in the dry exit gas	78.064	%

Notes for this case

• CO + H_2O ⍰ CO_2 + H_2 with K_p = exp(4577.8/T − 4.33) (Moe); equimolar, so pressure does not shift the equilibrium. Real reactors approach equilibrium within a margin set by catalyst activity (high-temperature shift about 350–450 °C, low-temperature about 200–250 °C).

Formula and method

$$K_p = \frac{y_{CO_2} y_{H_2}}{y_{CO} y_{H_2O}} = \exp\left(\frac{4577.8}{T} - 4.33\right)$$

Variables

T	Reactor exit temperature	K
n_{CO}	CO in feed (mol)	-
n_{H_2O}	Steam in feed (mol)	-
n_{CO_2}	CO_2 in feed (mol)	-
n_{H_2}	H_2 in feed (mol)	-
K_p	Equilibrium constant	-
X_{CO}	Equilibrium CO conversion	-
ξ	Extent of reaction (mol)	-
$y_{CO,dry}$	CO in the dry exit gas	-
$y_{H_2,dry}$	H_2 in the dry exit gas	-

Method and standards

Shift equilibrium.

Assumptions and limits

- Ideal gas; equilibrium reached; no methanation.

References

Water-gas shift equilibrium

Report details

Report reference	FCC-QRM2-E4AH (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/environmental/hydrogen-fuel-cells/water-gas-shift-equilibrium

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.