Activity Coefficient by the Davies Equation and Ionic Strength

Ionic strength from TDS or entered directly, and the Davies activity coefficient and activity of an ion of a given charge at a given temperature.

Input parameters

Unit system: SI

Parameter	Value	Unit
Ionic strength from	TDS ($I \approx 2.5 \times 10^{-5}$ TDS in mg/L)	
Ionic strength, mol/L (if entered)	0.010000	
Total dissolved solids (if used)	400.00	mg/L
Ion charge (absolute)	2.0000	
Temperature	25.000	°C
Relative permittivity of water (78.54 at 25 °C)	78.540	
Ion concentration, mol/L	0.001000	

Calculated results

Parameter	Value	Unit
Ionic strength used	0.010000	
Debye–Hückel constant A	0.50791	
Log activity coefficient	-0.17860	
Activity coefficient	0.66283	
Activity	6.6283e-04	

Notes for this case

- Davies (1962) extension of Debye–Hückel, good to an ionic strength of about 0.5 mol/L; the TDS estimate is Langelier's.

Formula and method

$$\log\gamma = -Az^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right), \quad A = 1.82\times10^{6}(\varepsilon_r T)^{-3/2}$$

$$I = \frac{1}{2}\sum C_i z_i^2 \approx 2.5\times10^{-5}\,TDS$$

Variables

I source	Ionic strength from	-
I	Ionic strength, mol/L (if entered)	-
TDS	Total dissolved solids (if used)	kg/m³
z	Ion charge (absolute)	-
T	Temperature	K
ε_r	Relative permittivity of water (78.54 at 25 °C)	-
C	Ion concentration, mol/L	-
A	Debye–Hückel constant A	-
$\log\gamma$	Log activity coefficient	-

γ	Activity coefficient	-
$\{C\}$	Activity	-

Method and standards

Davies activity coefficient model.

Assumptions and limits

- Dilute to moderately concentrated solutions.

Report details

Report reference	FCC-MJY5-G0EM (the same inputs always give the same reference)
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Calculator	Activity Coefficient by the Davies Equation and Ionic Strength
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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/drinking-water/activity-coefficient-davies

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.