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Topic 7.7: Calculating Equilibrium Concentrations

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UNIT 7 · EQUILIBRIUM

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The ICE Table Turns K into One Equation in x

Given K and a starting mixture, the equilibrium concentrations are the unknowns. The ICE table organises the bookkeeping in three rows: Initial (the starting concentrations), Change (written in terms of a single unknown, x), and Equilibrium (the initial row plus the change row).

Only the equilibrium row goes into the K expression. Substituting it gives one equation in one unknown; the rest of this topic is choosing a legal way to solve it.

The Change Row Carries the Coefficients

The variable x is the change in concentration tied to the extent of reaction. Each species changes by its own coefficient times x: reactants fall, products rise, and the mole ratio is preserved exactly.

For $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$ starting with $[N_2] = 0.40$, $[H_2] = 1.20$ and no NH_3, the equilibrium row is $[N_2] = 0.40 - x$, $[H_2] = 1.20 - 3x$, $[NH_3] = 2x$. If H_2 fell by only x, the row would destroy hydrogen atoms: each x of reaction consumes 3x of H_2 per x of N_2.

Products present at the start change nothing: they appear in the initial row, and their change entries still follow their coefficients.

Perfect Squares: Take the Square Root of Both Sides

Some expressions are a ratio of squares. When the equilibrium row produces $(2x)^2$ over $(a - x)^2$, taking the square root of both sides turns the equation into a linear one; no quadratic is needed.

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Watch for the pattern rather than the reaction: squared terms top and bottom. The square root step also produces a second, negative candidate value; it is tested like any other root.

The Quadratic Formula, and Rejecting Roots

When the expression is not a perfect square, expand it into the standard form $ax^2 + bx + c = 0$ and use the quadratic formula. Two roots come out, and algebra alone cannot choose between them.

A root is physical only if every equilibrium concentration stays positive and no species holds more atoms than the starting mixture supplied. A root that makes a concentration negative is discarded, however clean it looks. If both roots fail, the error is in the ICE table, usually a sign or a missing coefficient in the change row.

The Small-x Approximation and the 5 Percent Check

When K is very small, the reaction barely moves and x is tiny. A term like $(0.50 - x)$ can then be replaced by 0.50, and the equation collapses to something solvable by a square root.

The check that follows is not optional: x must be less than 5 percent of the concentration it was subtracted from. If it is, the neglected amount was genuinely negligible. If it is not, the quadratic must be solved instead. The approximation can even return an x larger than the starting concentration, which is impossible: no reactant can lose more than it had.

Check the Answer by Substituting Back

The finished equilibrium row, substituted into the K expression, must return the stated K within rounding. This check catches wrong roots, dropped coefficients and misread squares, because all of them disturb the ratio.

Two further checks cost nothing: no equilibrium concentration may be negative, and the atoms in the equilibrium row must match the atoms in the initial row. For a very large K the row shows reactants nearly, but never exactly, used up.

Worked Examples

Example 1: A perfect square. For $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$, Kc = 64.0, starting with $[H_2] = [I_2] = 0.50$ mol L^{-1} and no HI. The equilibrium row is $0.50 - x$, $0.50 - x$, $2x$, so $Kc = (2x)^2 / (0.50 - x)^2 = 64$. Taking square roots: $2x / (0.50 - x) = 8$, so $2x = 4.0 - 8x$ and $x = 0.40$. Then $[HI] = 0.80$ and $[H_2] = [I_2] = 0.10$ mol L^{-1}. Check: $(0.80)^2 / (0.10 \times 0.10) = 64$.

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Example 2: A quadratic, and a failed 5 percent check. For $PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$, Kc = 0.042, starting with $[PCl_5] = 1.00$ mol L^{-1}. The small-x estimate is $x = \sqrt{0.042} = 0.205$ M, which is 20.5 percent of 1.00 M, so the approximation fails. The full equation $x^2 / (1.00 - x) = 0.042$ rearranges to $x^2 + 0.042x - 0.042 = 0$, whose positive root is x = 0.185 M. Then $[PCl_5] = 0.815$ and $[PCl_3] = [Cl_2] = 0.185$ mol L^{-1}, an 18.5 percent dissociation. Check: $(0.185)^2 / 0.815 = 0.042$.

Example 3: A valid small-x approximation. For $SO_2Cl_2(g) \rightleftharpoons SO_2(g) + Cl_2(g)$, $Kc = 2.0 \times 10^{-5}$, starting with $[SO_2Cl_2] = 0.50$ mol L^{-1}. Neglecting x next to 0.50 gives $x^2 / 0.50 = 2.0 \times 10^{-5}$, so $x = \sqrt{(2.0 \times 10^{-5} \times 0.50)} = 3.2 \times 10^{-3}$. The check: 3.2×10^{-3} is 0.64 percent of 0.50, well under 5 percent, so the approximation stands and $[Cl_2] = [SO_2] = 3.2 \times 10^{-3}$ mol L^{-1}. The equilibrium $[SO_2Cl_2]$ is $0.50 - 0.0032 = 0.497$ mol L^{-1}.

Example 4: Both roots positive, one impossible. For $2NO_2(g) \rightleftharpoons N_2O_4(g)$, Kc = 25, starting with $[NO_2] = 0.60$ mol L^{-1} and no N_2O_4. The row is $[NO_2] = 0.60 - 2x$, $[N_2O_4] = x$, giving $x / (0.60 - 2x)^2 = 25$, or $100x^2 - 61x + 9 = 0$. The roots are x = 0.25 and x = 0.36, both positive. But x = 0.36 sets $[NO_2] = 0.60 - 0.72 = -0.12$ mol L^{-1}, so it is rejected: it consumes more NO_2 than the vessel holds. With x = 0.25, $[NO_2] = 0.10$ and $[N_2O_4] = 0.25$ mol L^{-1}. Check: $0.25 / (0.10)^2 = 25$.

Traps That Cost Marks in Topic 7.7

"Every species changes by x." Species change by their coefficient times x. In the ammonia synthesis the H_2 change is 3x, not x, and writing x breaks the atom balance of the whole table.

"Substitute the initial row into K." K is built from equilibrium concentrations only. The initial row gives Q at the first instant, and if a product starts absent that value is 0: a statement about direction, never a value of K.

"Neglect x whenever K looks small." The licence to neglect comes from the 5 percent check run after solving, not from the look of K. For $PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$ with Kc = 0.042 and $[PCl_5] = 1.00$ mol L^{-1}, neglecting x gives 20.5 percent dissociation; the check fails, and the quadratic gives 18.5 percent.

"Keep the smaller root, or the tidier root." Roots are chosen by the equilibrium row, not by size or neatness. Keep the root that leaves every concentration positive and reachable; if both fail, rebuild the ICE table.

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"$(2x)^2$ can be written as $2x^2$." The whole concentration is squared: $(2x)^2 = 4x^2$. Writing $2x^2$ understates the product term by a factor of 2 and shifts the solved x with it.

"A huge K means the reaction goes to completion, so no solving is needed." Equilibrium still leaves a trace of reactant. For $H_2(g) + Br_2(g) \rightleftharpoons 2HBr(g)$ with $K_c = 3.8 \times 10^4$ and both reactants at 0.10 mol L^{-1}, the square root method gives [HBr] = 0.198 mol L^{-1} with 0.0010 mol L^{-1} of each reactant left, not 0.20 and zero.

Key Relationships to Remember

- ICE rows: equilibrium = initial + change, and only the equilibrium row enters the K expression
- Every change entry is the species coefficient times x, negative for reactants and positive for products in the direction written
- A ratio of squares in the K expression is solved by taking the square root of both sides, giving a linear equation
- A non-square expression is expanded to $ax^2 + bx + c = 0$ and solved with the quadratic formula
- A root is accepted only when every equilibrium concentration it produces is positive and atom-balanced against the initial row
- The small-x approximation replaces $(c - x)$ with c, valid only when x is under 5 percent of c
- A failed 5 percent check, or an approximate x larger than the starting concentration, sends the problem back to the quadratic
- The solved equilibrium row must return the stated K on back-substitution; that check closes every problem in this topic

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Topic 7.7 Quiz: Calculating Equilibrium Concentrations

Topic 7.7 Worksheet

Unit 7: All Topics

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