

Estimate the final volume of a mixture when 34 mL of water is added to 66 mL of ethanol.

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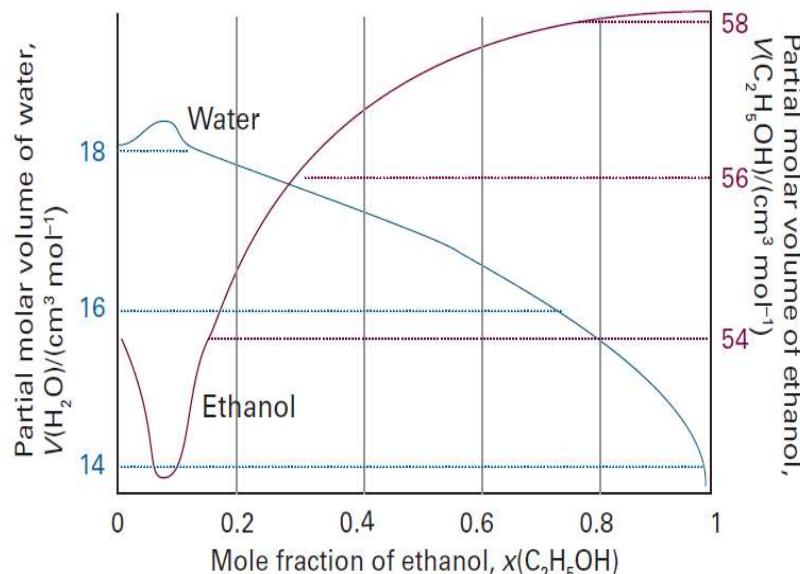
> restart;
> ρW, ρEtOH := 1, 0.7893 : # densities in g/
> MW, MEtOH := 18.01, 46.07 : # molecular weights in g/mol
# Values taken from <https://en.wikipedia.org/wiki/Ethanol\_\(data\_page\)>

> VW, VEtOH := 34, 66 : # volumes in mL
> nW :=  $\frac{V_W \cdot \rho_W}{M_W}$  : # moles of water
> nEtOH :=  $\frac{V_{EtOH} \cdot \rho_{EtOH}}{M_{EtOH}}$  : # moles of EtOH
> xEtOH :=  $\frac{n_{EtOH}}{n_{EtOH} + n_W}$ ; # molar fraction of EtOH
0.3746

```

(1.1)

Partial molar volumes of water and ethanol at 25 °C, Atkins p.181



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> V-W, V-EtOH := 17.5, 57 : # partial volumes in mL/mol,
approximated from the graph
> V := nW·V-W + nEtOH·V-EtOH; # total volume of mixture in mL
97.4901

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(1.2)

For a chemical reaction, $3A(g) = 4B(g)$, calculate the change in the fraction of A molecules dissociated if the reaction pressure is tripled

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> restart;
> nA := n·(1 - 3 · alpha) : # number of moles of A at equilibrium,
  assuming there are "n" moles of A to begin with
> nB := 4·alpha·n : # number of moles of B at equilibrium, assuming
  there are 0 moles of B at the beginning
> xA := simplify( $\left(\frac{n_A}{n_A + n_B}\right)$ ); # mol fraction of A

$$x_A := \frac{1 - 3\alpha}{1 + \alpha} \quad (2.1)$$


> xB := simplify( $\left(\frac{n_B}{n_A + n_B}\right)$ ); # mol fraction of B

$$x_B := \frac{4\alpha}{1 + \alpha} \quad (2.2)$$


> eq := KP =  $\frac{(x_B \cdot P)^4}{(x_A \cdot P)^3}$ ; # equilibrium constant for the reaction

$$eq := K_P = \frac{256\alpha^4 P}{(1 + \alpha)(1 - 3\alpha)^3} \quad (2.3)$$


> eqS := lhs(eq) = rhs(eq) · (1 + alpha) · (1 - 3 · alpha)3; # by assuming
  alpha << 1

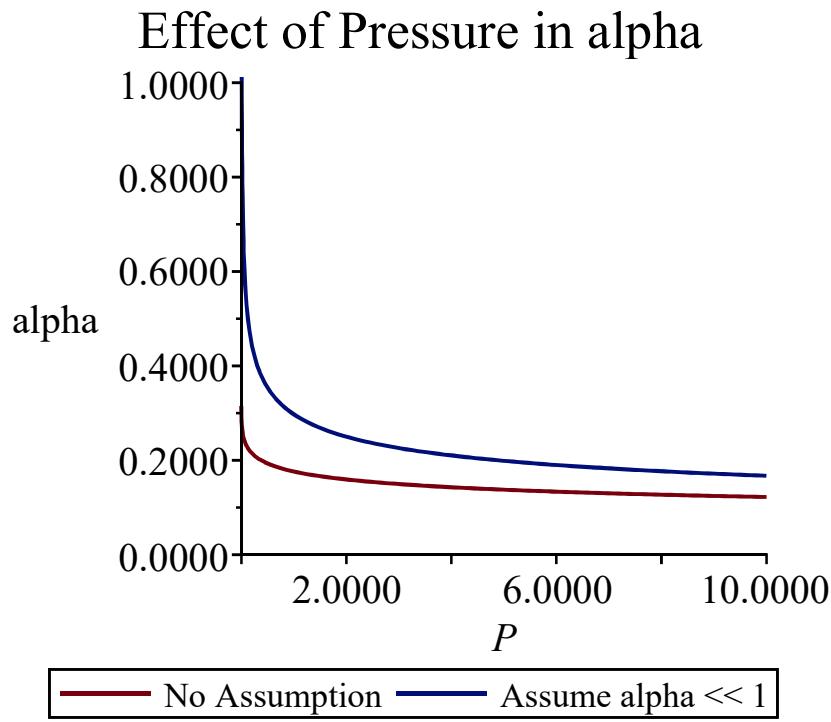
$$eqS := K_P = 256\alpha^4 P \quad (2.4)$$


> alphaF := solve(eq, alpha, explicit )[3]: # solve for the real,
  positive solution for alphaF and alphas
alphas := solve(eqS, alpha, explicit )[1]

$$\alpha_{ph} := \frac{\left(\frac{K_P}{P}\right)^{1/4}}{4} \quad (2.5)$$

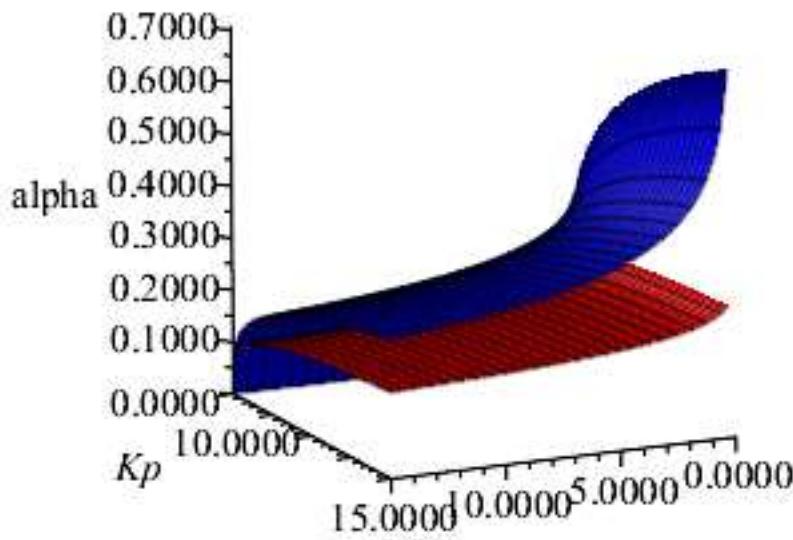

> plots[animate](plot, [[alphaF, alphas], P], KP = 0 .. 2)
  # letting KP vary, we plot both alphas
  # we can observe that alpha decreases as P increases, as per Le
  Chatelier's law.

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> # for a more general idea, we can also make a 3 D plot; note
  that it is a mirror image of the plot above for easier
  visualization
plot3d([alphaF(P, Kp), alphaS(P, Kp)], P = 0 .. 15, Kp = 0 .. 20, color
  = ["Red", "Blue"])
```

Alpha as a function of Kp and Pressure



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>  $\alpha_2 := \text{subs}(P = 3 \cdot P, \text{alphaF})$  : # solve for alpha when the pressure
   is tripled
> plots[animate](plot, [subs( $K_p = \text{rhs}(\text{eq})$ ,  $\alpha_2$ ), alpha], P=0..2)
   # letting P vary, we plot the alphas against each other
   (note that the relationship is not a function of P, P just
   has to be  $> 0$ )

```

