

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

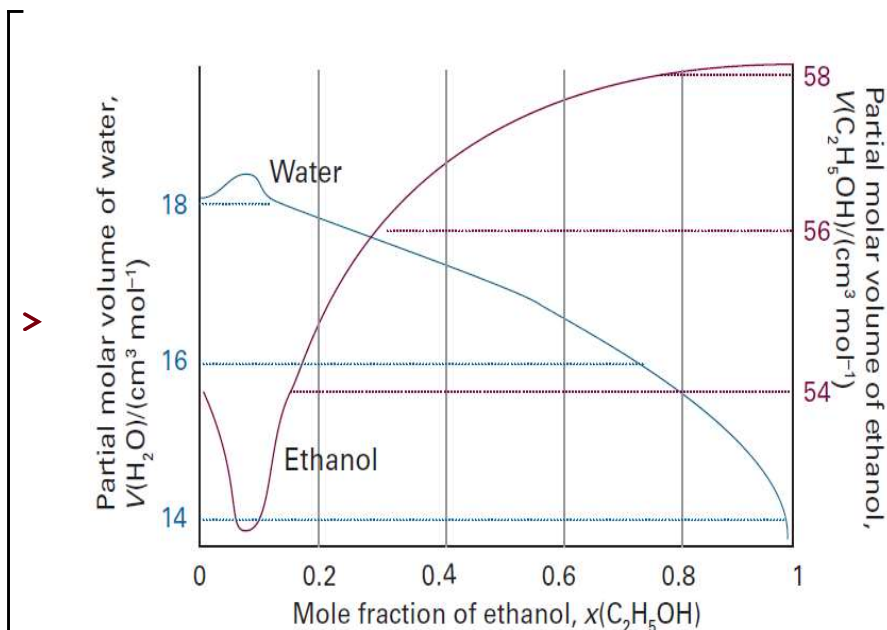
```

> restart;
>  $\rho_W$  ,  $\rho_{EtOH}$  := 1, 0.7893 : # densities in g/
>  $M_W$  ,  $M_{EtOH}$  := 18.01, 46.07 : # molecular weights in g/mol
  # Values taken from <https://en.wikipedia.org/wiki/Ethanol\_\(data\_page\)>
>  $V_W$  ,  $V_{EtOH}$  := 34, 66 : # volumes in mL
>  $n_W := \frac{V_W \cdot \rho_W}{M_W}$  : # moles of water
>  $n_{EtOH} := \frac{V_{EtOH} \cdot \rho_{EtOH}}{M_{EtOH}}$  : # moles of EtOH
>  $x_{EtOH} := \frac{n_{EtOH}}{n_{EtOH} + n_W}$  ; # molar fraction of EtOH

```

0.3746 (1.1)

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



```

>  $V_W$  ,  $V_{-EtOH}$  := 17.5, 57 : # partial volumes in mL/mol,
  approximated from the graph
>  $V := n_W \cdot V_W + n_{EtOH} \cdot V_{-EtOH}$  ; # total volume of mixture in mL

```

97.4901 (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

```
> restart;
```

```
> n_A := n*(1 - 3*alpha): # number of moles of A at equilibrium,
    assuming there are "n" moles of A to begin with
```

```
> n_B := 4*alpha*n: # number of moles of B at equilibrium, assuming
    there are 0 moles of B at the beginning
```

```
> x_A := simplify( (n_A / (n_A + n_B)) ); # mol fraction of A
```

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

```
> x_B := simplify( (n_B / (n_A + n_B)) ); # mol fraction of B
```

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

```
> eq := Kp = (x_B*P)^4 / (x_A*P)^3; # equilibrium constant for the reaction
```

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

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

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

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

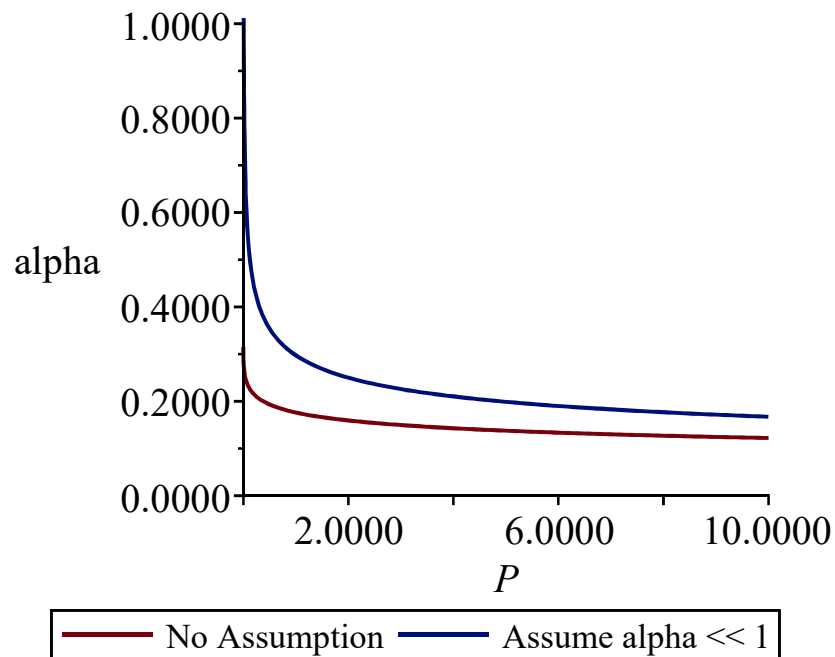
$$\alpha_S := \frac{\left(\frac{Kp}{P}\right)^{1/4}}{4} \quad (2.5)$$

```
> plots[animate](plot, [[alphaF, alphaS], P], Kp=0..2)
```

```
    # letting Kp vary, we plot both alphas
```

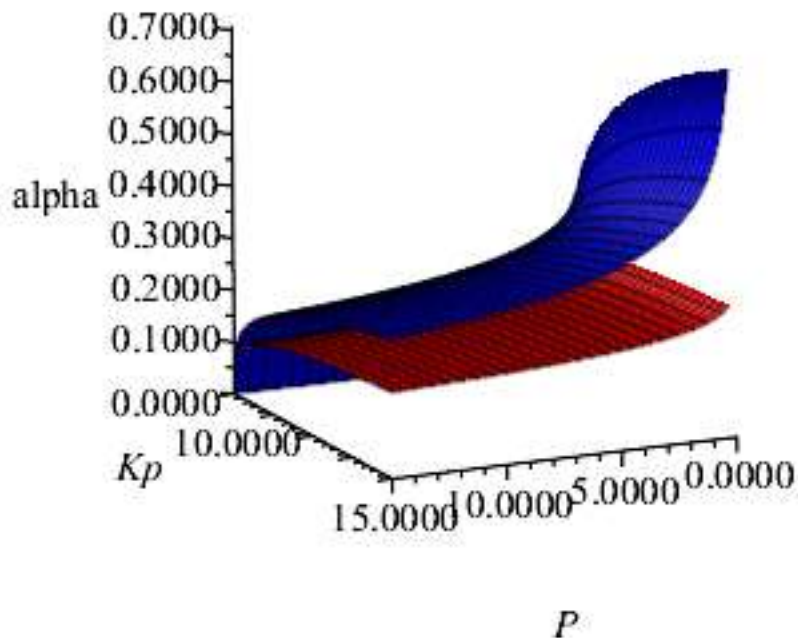
```
    # we can observe that alpha decreases as P increases, as per Le
    Chatelier's law.
```

Effect of Pressure in alpha



```
> # 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



```

>  $\alpha_2 := \text{subs}(P = 3 \cdot P, \text{alphaF}) : \# \text{ solve for alpha when the pressure}$ 
   $\text{is tripled}$ 
> plots[animate](plot, [subs( $Kp = \text{rhs}(eq)$ ,  $\alpha_2$ ), 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)

```

