With the explicit expressions - ideal gas

```
In[ ]:= kB = 1.380649 × 10^-23;(*J/K*)
        h = 6.62607015 × 10^-34; (*J/Hz*)
        Da = 1.66053906660 × 10^-27;(*kg*)

In[ ]:= κnum = 100; κmin = 0.5; κmax = 2; Ratios4κ = Table[{}, {i, 1, κnum + 1}];

        For[j = 1, j ≤ κnum + 1, j++,
          κ = κmin + (j - 1) (κmax - κmin) / κnum;  (*=m2/m1*)
          u = 0;
          m2 = 10 Da; (*mass of a molecule*)
          (*mixture state variables*)
          ρ = 1;  (*kg/m^3*)
          u = 0 × 10^3;  (*kg m/s*)
          (*set either energy or temperature*)
          e = 3/2 kB 300 (ρ/m2) + 1/2 u^2/ρ;  (*J/m^3*)(*some reasonable
           estimate of total mixture energy; Note that with u=0 we have e=ϵ,
          that is total mixture energy is equal to internal mixture energy*)
          (*T=300;(*K*) *)
          rel26 = κ^(5/2 κ) m2^(4 (1-κ)) ρ1^κ (4 π/3 (e - u^2/(2 ρ))/(h^2 (κ ρ1 + ρ - ρ1)))^(3/2 (1-κ))        ;
          rel24 = (2 e ρ^2 + u^2 (κ^-1 - 1) (ρ - ρ1))/(2 ρ (ρ1 + κ^-1 (ρ - ρ1))) ρ1/ρ;
          rel23 = ρ1/ρ u;
          ρ1sol = FindRoot[ρ - ρ1 == rel26, {ρ1, 0.5 ρ}] // Flatten;
          e1sol = FindRoot[e1 == rel24 /. ρ1sol, {e1, 0.5 e}] // Flatten;
          u1sol = FindRoot[u1 == ρ1/ρ u /. ρ1sol, {u1, 0.5 u}] // Flatten;
          ρ2sol = {ρ2 → ((ρ - ρ1) /. ρ1sol)};
          e2sol = {e2 → (e - e1 /. e1sol)};
```

$$\text{u2sol} = \left\{u2 \to \left(\frac{\rho 2}{\rho}\ u\ /.\ \rho 2\text{sol}\right)\right\};$$

$$\text{s1sol} = \left\{s1 \to \left(kB\ \frac{\rho 1}{m1}\left(\frac{5}{2} + \text{Log}\left[\frac{m1}{\rho 1}\left(\frac{4\,\pi\,m1}{3\,h^2}\ \frac{e1 - \frac{u1^2}{2\,\rho 1}}{\rho 1\,/\,m1}\right)^{3/2}\right]\right)\right)/.\ m1 \to m2\,\kappa^{-1}\ /.\ \rho 1\text{sol}\ /.\ \text{u1sol}\ /.\ \text{e1sol}\right\};$$

$$\text{s2sol} = \left\{s2 \to \left(kB\ \frac{\rho 2}{m2}\left(\frac{5}{2} + \text{Log}\left[\frac{m2}{\rho 2}\left(\frac{4\,\pi\,m2}{3\,h^2}\ \frac{e2 - \frac{u2^2}{2\,\rho 2}}{\rho 2\,/\,m2}\right)^{3/2}\right]\right)\right)/.\ \rho 2\text{sol}\ /.\ \text{u2sol}\ /.\ \text{e2sol}\right\};$$

$$\rho\text{star} = -\frac{kB}{m1}\,\text{Log}\left[\frac{\rho 1}{m1}\right] + \frac{3}{2}\,\frac{kB}{m1}\,\text{Log}\left[\frac{4\,\pi\,m1}{3\,h^2}\,\frac{m1}{\rho 1}\left(e1 - \frac{u1^2}{2\,\rho 1}\right)\right] + \frac{3}{2}\,\frac{kB}{m1}\,\frac{1}{e1 - \frac{u1^2}{2\,\rho 1}}\,\frac{u1^2}{2\,\rho 1}\ /.\ m1 \to m2\,\kappa^{-1}\ /.\ \rho 1\text{sol}\ /.\ \text{u1sol}\ /.\ \text{e1sol};$$

$$\text{estar} = D\left[\left(kB\ \frac{\rho 1}{m1}\left(\frac{5}{2} + \text{Log}\left[\frac{m1}{\rho 1}\left(\frac{4\,\pi\,m1}{3\,h^2}\ \frac{e1 - \frac{u1^2}{2\,\rho 1}}{\rho 1\,/\,m1}\right)^{3/2}\right]\right)\right),\ e1\right]/.\ m1 \to m2\,\kappa^{-1}\ /.\ \rho 1\text{sol}\ /.\ \text{u1sol}\ /.\ \text{e1sol};$$

```
p = (-e + ρ μ + T s) /. μ → (-ρstar T) /. T → 1 / estar /. s → s1 + s2 /. ρ1sol /. e1sol /. s1sol /.
  s2sol;
p1 = -e1 + ρ1 μ + T s1 /. μ → (-ρstar T) /. T → 1 / estar /. e1sol /. ρ1sol /. s1sol;
p2 = -e2 + ρ2 μ + T s2 /. μ → (-ρstar T) /. T → 1 / estar /. e2sol /. ρ2sol /. s2sol;
```

$$\text{Ratios4}\kappa[[j]] = \left\{\kappa,\ \text{Chop}[\rho 1\,/\,\rho\ /.\ \rho 1\text{sol}],\ \text{Chop}\left[\left(\frac{\rho 1}{\rho}\ e\,/\,e1\right)/.\ \rho 1\text{sol}\ /.\ \text{e1sol}\right],\right.$$

$$\text{Chop}\left[\left(\frac{\rho 1}{\rho}\ s\,/\,s1\right)/.\ s \to s1 + s2\ /.\ \rho 1\text{sol}\ /.\ \text{s1sol}\ /.\ \text{s2sol}\right],$$

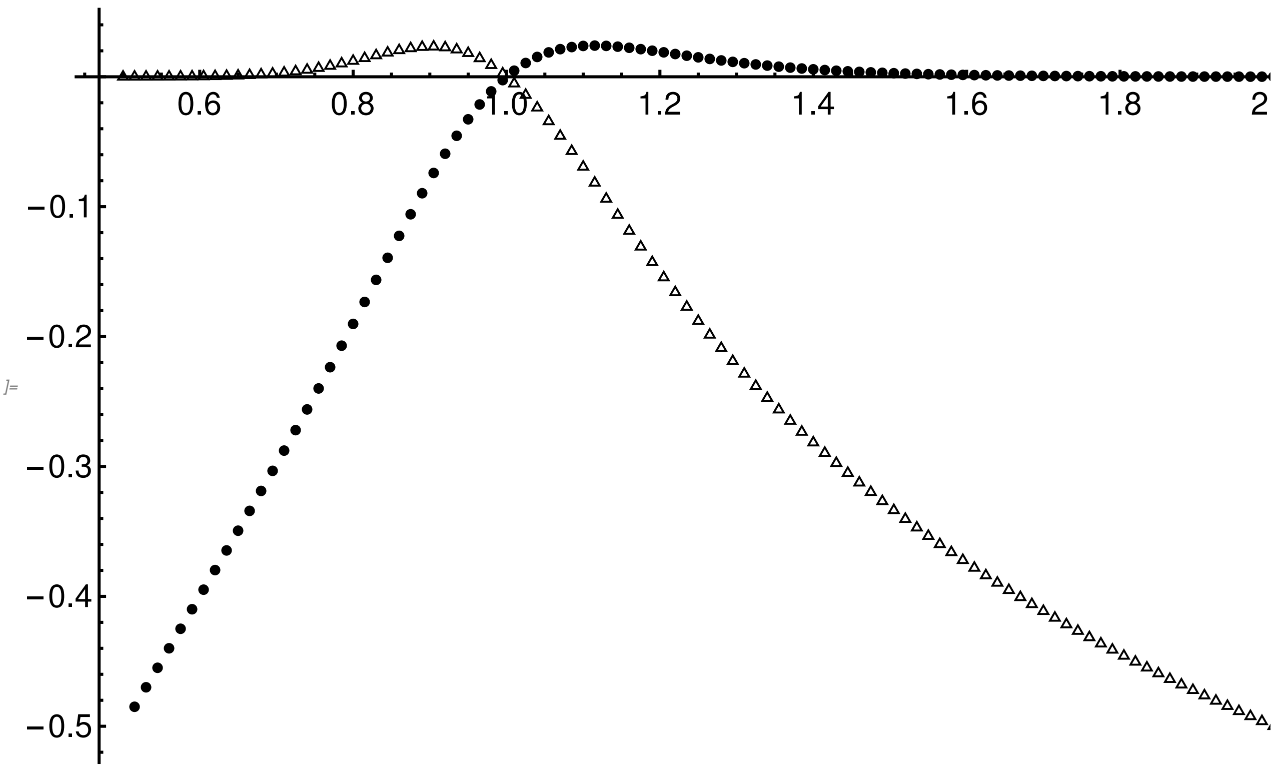
$$\text{Chop}\left[\left(\left(\frac{\rho 1}{\rho}\ e - e1\right) - T\left(\frac{\rho 1}{\rho}\ s - s1\right)\right)\Big/\left(\frac{\rho 1}{\rho}\ p\right)/.\ s \to s1 + s2\ /.\ \rho 1\text{sol}\ /.\ \text{e1sol}\ /.\ \text{s1sol}\ /.\ \text{s2sol}\right],$$

```
  Chop[(ρ1) /. ρ1sol], Chop[(ρ2) /. ρ2sol], Chop[(e1) /. e1sol], Chop[(e2) /. e2sol],
  Chop[(s1) /. s1sol], Chop[(s2) /. s2sol], Chop[p], Chop[p1], Chop[p2], Chop[estar]}];
```

```
In[ ]:= Clear[κ, j, p, p1, p2, estar];
```

```
In[ ]:= ListPlot[{Table[{Ratios4κ[[j, 1]],
      Chop[((ρ1/ρ (e1 + e2) - e1) - 1/estar (ρ1/ρ (s1 + s2) - s1))/(ρ1/ρ p) /. ρ1 → Ratios4κ[[j, 6]] /.
              ρ2 → Ratios4κ[[j, 7]] /. e1 → Ratios4κ[[j, 8]] /. e2 → Ratios4κ[[j, 9]] /.
          s1 → Ratios4κ[[j, 10]] /. s2 → Ratios4κ[[j, 11]] /. p → Ratios4κ[[j, 12]] /.
        p1 → Ratios4κ[[j, 13]] /. p2 → Ratios4κ[[j, 14]] /. estar → Ratios4κ[[j, 15]],
      10^-8]}, {j, 1, κnum + 1}], Table[{Ratios4κ[[j]][[1]],
      Chop[((ρ2/ρ (e1 + e2) - e2) - 1/estar (ρ2/ρ (s1 + s2) - s2))/(ρ2/ρ p) /. ρ1 → Ratios4κ[[j, 6]] /.
              ρ2 → Ratios4κ[[j, 7]] /. e1 → Ratios4κ[[j, 8]] /. e2 → Ratios4κ[[j, 9]] /.
          s1 → Ratios4κ[[j, 10]] /. s2 → Ratios4κ[[j, 11]] /. p → Ratios4κ[[j, 12]] /.
        p1 → Ratios4κ[[j, 13]] /. p2 → Ratios4κ[[j, 14]] /. estar → Ratios4κ[[j, 15]], 10^-8]},
    {j, 1, κnum + 1}]}, AxesStyle → Thickness[0.0025], PlotTheme →
   {"Monochrome"},
  LabelStyle →
   {FontSize → 16,
    Black},
  AxesLabel → {Style["κ"(*"\kappa"*),
     FontFamily → "Times", FontSize → 20]}]
```

Out[ ]=

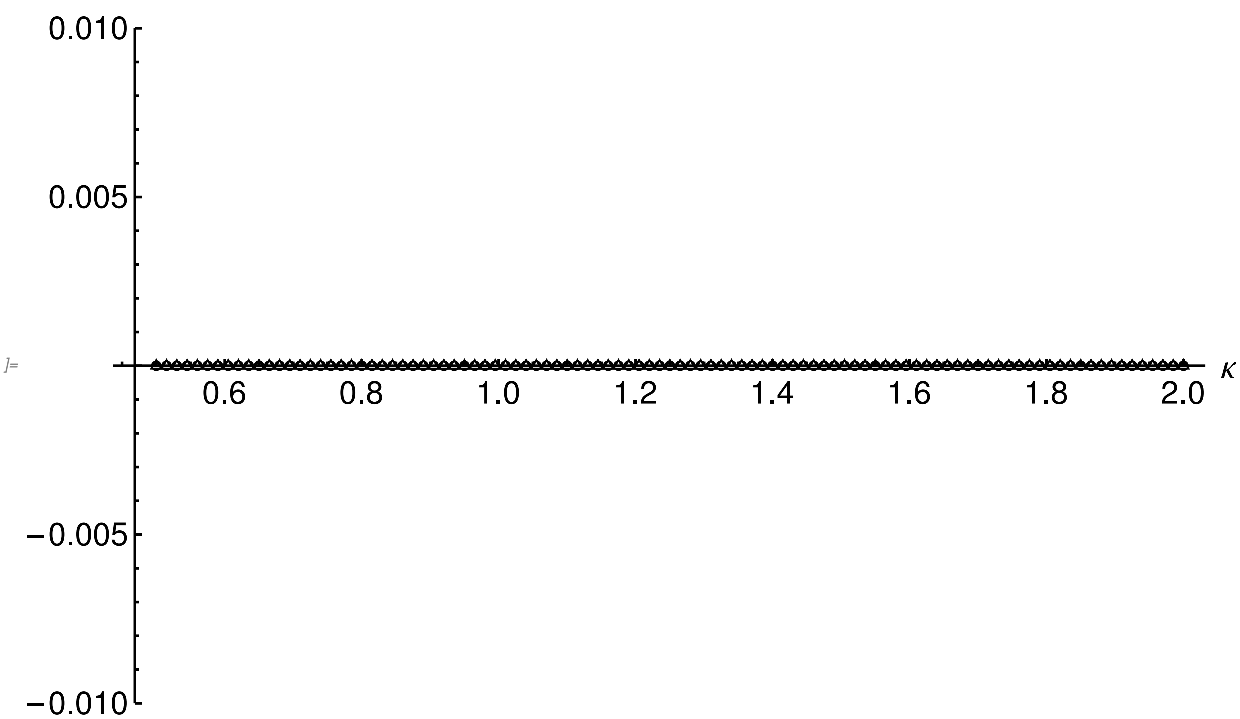


index 1 is denoted with circles, index 2 with triangles

Testing Dalton’s law of partial pressures, distribution according to $(p_\alpha - x_\alpha\ p)/(x_\alpha\ \mathrm{p})$

In[ ]:=
```
ListPlot[{Table[{Ratios4κ[[j, 1]],
    Chop[(p1 - ρ1/(ρ1 + κ^-1 ρ2) p)/(ρ1/(ρ1 + κ^-1 ρ2) p) /. κ → Ratios4κ[[j, 1]] /. ρ1 → Ratios4κ[[j, 6]] /.
          ρ2 → Ratios4κ[[j, 7]] /. e1 → Ratios4κ[[j, 8]] /. e2 → Ratios4κ[[j, 9]] /.
        s1 → Ratios4κ[[j, 10]] /. s2 → Ratios4κ[[j, 11]] /. p → Ratios4κ[[j, 12]] /.
      p1 → Ratios4κ[[j, 13]] /. p2 → Ratios4κ[[j, 14]] /. estar → Ratios4κ[[j, 15]],
   10^-8]}, {j, 1, κnum + 1}], Table[{Ratios4κ[[j, 1]],
    Chop[(p2 - κ^-1 ρ2/(ρ1 + κ^-1 ρ2) p)/(κ^-1 ρ2/(ρ1 + κ^-1 ρ2) p) /. κ → Ratios4κ[[j, 1]] /. ρ1 → Ratios4κ[[j, 6]] /.
          ρ2 → Ratios4κ[[j, 7]] /. e1 → Ratios4κ[[j, 8]] /. e2 → Ratios4κ[[j, 9]] /.
        s1 → Ratios4κ[[j, 10]] /. s2 → Ratios4κ[[j, 11]] /. p → Ratios4κ[[j, 12]] /.
      p1 → Ratios4κ[[j, 13]] /. p2 → Ratios4κ[[j, 14]] /. estar → Ratios4κ[[j, 15]], 10^-8]},
  {j, 1, κnum + 1}]}, AxesStyle → Thickness[0.0025], PlotTheme →
 {"Monochrome"},
 LabelStyle →
 {FontSize → 16,
  Black},
 AxesLabel → {Style["κ"(*"\kappa"*), FontFamily → "Times",
    FontSize → 20]}, PlotRange → {-0.01, 0.01}]
```

Out[ ]=



(numerically) Without the explicit expressions - ideal gas

In[ ]:= $s1 = kB \frac{\rho 1}{m1} \left(\frac{5}{2} + \mathrm{Log}\left[\frac{m1}{\rho 1} \left(\frac{4 \pi\, m1}{3\, h^2} \frac{e1 - \frac{u1^2}{2 \rho 1}}{\rho 1 / m1} \right)^{3/2} \right] \right);$

$s2 = kB \frac{\rho 2}{m2} \left(\frac{5}{2} + \mathrm{Log}\left[\frac{m2}{\rho 2} \left(\frac{4 \pi\, m2}{3\, h^2} \frac{e2 - \frac{u2^2}{2 \rho 2}}{\rho 2 / m2} \right)^{3/2} \right] \right);$

```
s = s1 + s2;
```

```
In[ ]:= FirstMEstep = {D[s, ρ1] == ρstar, D[s, ρ2] == ρstar, D[s, u1] == ustar,
    D[s, u2] == ustar, D[s, e1] == estar, D[s, e2] == estar} // Simplify;
```

instead of the second step, we use the upscaling mapping

```
In[ ]:= Projections = {ρ == ρ1 + ρ2, u == u1 + u2, e == e1 + e2};
```

```
In[ ]:= kB = 1.380649 × 10^-23;(*J/K*)
h = 6.62607015 × 10^-34; (*J/Hz*)
Da = 1.66053906660 × 10^-27;(*kg*)
```

With a prescribed energy:

```
κnum = 100;
κmin = 0.5;
κmax = 2;
Ratios4κ = Table[{}, {i, 1, κnum + 1}];
Clear[j, p, p1, p2, e, T, estar, κ, m1, m2];
For[j = 1, j ≤ κnum + 1, j++,
  κ = κmin + (j - 1) (κmax - κmin) / κnum;
  m2 = 10 Da; (*mass of a molecule*)
  m1 = m2 / κ;  (*κ=m2/m1*)
  (*mixture state variables*)
  ρ = 1;  (*kg/m^3*)
  u = 0 × 10^3;  (*kg m/s*)
  e = 3/2 kB 300 (ρ/m2) + 1/2 u^2/ρ;  (*J/m^3*)
  (*some reasonable estimate of total mixture energy from a prescribed temperature;
  again, internal and total are equal*)
  numEstimate = Chop[FindRoot[FirstMEstep ∪ Projections,
     {{ρ1, ρ (1.5 (κ - 0.45))}, {ρ2, ρ (1 - (1.5 (κ - 0.45)))}, {u1, u / 2}, {u2, u / 2},
      {e1, e / 2}, {e2, e / 2}, {ρstar, 10^3}, {ustar, 1}, {estar, 1 / 300}}]];
  p = (-e + ρ μ + T s) /. μ → (-ρstar T) /. T → 1 / estar /. numEstimate;
  p1 = -e1 + ρ1 μ + T s1 /. μ → (-ρstar T) /. T → 1 / estar /. numEstimate;
  p2 = -e2 + ρ2 μ + T s2 /. μ → (-ρstar T) /. T → 1 / estar /. numEstimate;
  Ratios4κ[[j]] =
   {κ, ρ1 /. numEstimate, ρ2 /. numEstimate, u1 /. numEstimate, u2 /. numEstimate,
    e1 /. numEstimate, e2 /. numEstimate, p, p1, p2, 1 / estar /. numEstimate}];
```

```
In[ ]:= Clear[j, p, p1, p2, m1, κ, estar]
```

```
In[ ]:= ListPlot[Table[{Ratios4κ[[j, 1]],
     ((ρ1/ρ (e1 + e2) - e1) - T (ρ1/ρ s - s1)) / (ρ1/ρ p) /. m1 → m2 / Ratios4κ[[j, 1]] /. T → 1 / estar /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
       u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
    p → Ratios4κ[[j, 8]]  /. estar → Ratios4κ[[j, 11]]}, {j, 1, κnum + 1}],
  AxesLabel → {"κ", "((ρ1/ρ e-e1)-T(ρ1/ρ s-s1))/(ρ1/ρ p) ratio"}
```

```
 (*,
 MaxPlotPoints→60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
   ((ρ2/ρ (e1 + e2) - e2) - T (ρ2/ρ s - s2)) / (ρ2/ρ p) /. m1 → m2 / Ratios4κ[[j, 1]] /. T → 1 / estar /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
        u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
     p → Ratios4κ[[j, 8]]  /. estar → Ratios4κ[[j, 11]]}, {j, 1, κnum + 1}],
 AxesLabel → {"κ", "((ρ2/ρ e-e2)-T(ρ2/ρ s-s2))/(ρ2/ρ p) ratio"}
 (*,
 MaxPlotPoints→60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
   (p1 - (ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
        u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
      p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
  {j, 1, κnum + 1}], AxesLabel → {"κ", "(p1 - x1 p) / (x1 p)"}
 (*,MaxPlotPoints→
  60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
   (p2 - (ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
        u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
      p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
  {j, 1, κnum + 1}], AxesLabel → {"κ", "(p2 - x2 p) / (x2 p)"}
 (*,MaxPlotPoints→
  60*)]
```

With a prescribed temperature:

```
κnum = 100;
κmin = 0.5;
κmax = 2;
Ratios4κ = Table[{}, {i, 1, κnum + 1}];
Clear[j, p, p1, p2, e, T, estar, κ, m1, m2];
For[j = 1, j ≤ κnum + 1, j++,
  κ = κmin + (j - 1) (κmax - κmin) / κnum;
  m2 = 10 Da; (*mol mass*)
  m1 = m2 / κ;  (*κ=m2/m1*)
  (*mixture state variables*)
  ρ = 1;  (*kg/m^3*)
  u = 0 × 10^3;  (*kg m/s*)
  T = 300;  (*K*)
  estar = 1 / T;
  eestimate = 3/2 kB / estar (ρ/((m1 + m2) / 2)) + 1/2 u^2/ρ; (*with u=0, total=internal*)
  numEstimate =
   Chop[FindRoot[FirstMEstep ∪ Projections, {{ρ1, ρ / 2}, {ρ2, ρ / 2}, {u1, u / 2}, {u2, u / 2},
      {e1, eestimate / 2}, {e2, eestimate / 2}, {ρstar, 10^3}, {ustar, 1}, {e, eestimate}}]];
  p = (-e + ρ μ + T s) /. μ → (-ρstar T) /. numEstimate;
  p1 = -e1 + ρ1 μ + T s1 /. μ → (-ρstar T) /. numEstimate;
  p2 = -e2 + ρ2 μ + T s2 /. μ → (-ρstar T) /. numEstimate;
  Ratios4κ[[j]] = {κ, ρ1 /. numEstimate, ρ2 /. numEstimate, u1 /. numEstimate,
    u2 /. numEstimate, e1 /. numEstimate, e2 /. numEstimate, p, p1, p2}];
```

```
In[ ]:= Clear[j, p, p1, p2, m1, κ, estar]
```

```
In[ ]:= ListPlot[Table[{Ratios4κ[[j, 1]],
    (((ρ1/ρ (e1 + e2) - e1) - T (ρ1/ρ s - s1))/(ρ1/ρ p) /. m1 → m2 / Ratios4κ[[j, 1]] /. ρ1 → Ratios4κ[[j,
            2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /. u2 → Ratios4κ[[j, 5]] /.
       e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /. p → Ratios4κ[[j, 8]]},
   {j, 1, κnum + 1}], AxesLabel → {"κ", "((ρ1/ρ e-e1)-T(ρ1/ρ s-s1))/(ρ1/ρ p) ratio"}
  (*,MaxPlotPoints→60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
```

```
(((ρ2/ρ) (e1 + e2) - e2) - T ((ρ2/ρ) s - s2)) / ((ρ2/ρ) p) /. m1 → m2 / Ratios4κ[[j, 1]] /. ρ1 → Ratios4κ[[j,
        2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /. u2 → Ratios4κ[[j, 5]] /.
    e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /. p → Ratios4κ[[j, 8]]},
  {j, 1, κnum + 1}], AxesLabel → {"κ", "(((ρ2/ρ) e-e2)-T((ρ2/ρ) s-s2))/((ρ2/ρ) p) ratio"}
 (*,MaxPlotPoints→60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
   (p1 - (ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
        ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
      u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
    p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
  {j, 1, κnum + 1}], AxesLabel → {"κ", "(p_1 - x_1 p) / (x_1 p)"}
 (*,MaxPlotPoints→
  60*)]
ListPlot[Table[{Ratios4κ[[j, 1]],
   (p2 - (ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
        ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
      u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
    p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
  {j, 1, κnum + 1}], AxesLabel → {"κ", "(p_2 - x_2 p) / (x_2 p)"}
 (*,MaxPlotPoints→
  60*)]
```

matches the explicit results

Without the explicit expressions - vdW gas

In[ ]:=
$$s1 = \frac{3}{2}\frac{kB}{m1}\rho1\,\text{Log}\left[\frac{T1}{Tref}\right] - \frac{kB}{m1}\rho1\,\text{Log}\left[C1\frac{\rho1/m1}{1-v1\,\rho1/m1}\right] /.\ T1 \to \left(e1 - \frac{1}{2}\frac{u1^2}{\rho1} - a1\,\rho1^2\right)\left(\frac{3}{2}\frac{kB}{m1}\rho1\right)^{-1};$$
$$s2 = \frac{3}{2}\frac{kB}{m2}\rho2\,\text{Log}\left[\frac{T2}{Tref}\right] - \frac{kB}{m2}\rho2\,\text{Log}\left[C2\frac{\rho2/m2}{1-v2\,\rho2/m2}\right] /.\ T2 \to \left(e2 - \frac{1}{2}\frac{u2^2}{\rho2} - a2\,\rho2^2\right)\left(\frac{3}{2}\frac{kB}{m2}\rho2\right)^{-1};$$

```
s = s1 + s2;
```

In[ ]:=
```
FirstMEstep = {D[s, ρ1] == ρstar, D[s, ρ2] == ρstar, D[s, u1] == ustar,
    D[s, u2] == ustar, D[s, e1] == estar, D[s, e2] == estar} // Simplify;
```

instead of the second step, we use projections

In[ ]:=
```
Projections = {ρ == ρ1 + ρ2, u == u1 + u2, e == e1 + e2};
(*free ene fE=e-Ts; pressure p=ρ ∂ρfE-fE*)
```

$$fE = \frac{3}{2}\frac{kB}{m}\rho\,T + \frac{1}{2}\frac{u^2}{\rho} - a\,\rho^2 - T\left(\frac{3}{2}\frac{kB}{m}\rho\,\text{Log}\left[\frac{T}{Tref}\right] - \frac{kB}{m}\rho\,\text{Log}\left[C\frac{\rho/m}{1-v\,\rho/m}\right]\right) \text{ // Simplify}$$

```
ρ D[fE, ρ] - fE // Simplify
```

Out[ ]=
$$\frac{m\,u^2 + 3\,kB\,T\,\rho^2 - 2\,a\,m\,\rho^3 - 3\,kB\,T\,\rho^2\,\text{Log}\left[\frac{T}{Tref}\right] + 2\,kB\,T\,\rho^2\,\text{Log}\left[\frac{C\,\rho}{m-v\,\rho}\right]}{2\,m\,\rho}$$

Out[ ]=
$$\frac{m\left(u^2 + a\,\rho^3\right) - \rho\left(u^2\,v + kB\,T\,\rho + a\,v\,\rho^3\right)}{\rho\left(-m + v\,\rho\right)}$$

In[ ]:=
```
% /. u → 0 // Simplify
```

Out[ ]=
$$\rho\left(-a\,\rho + \frac{kB\,T}{m - v\,\rho}\right)$$

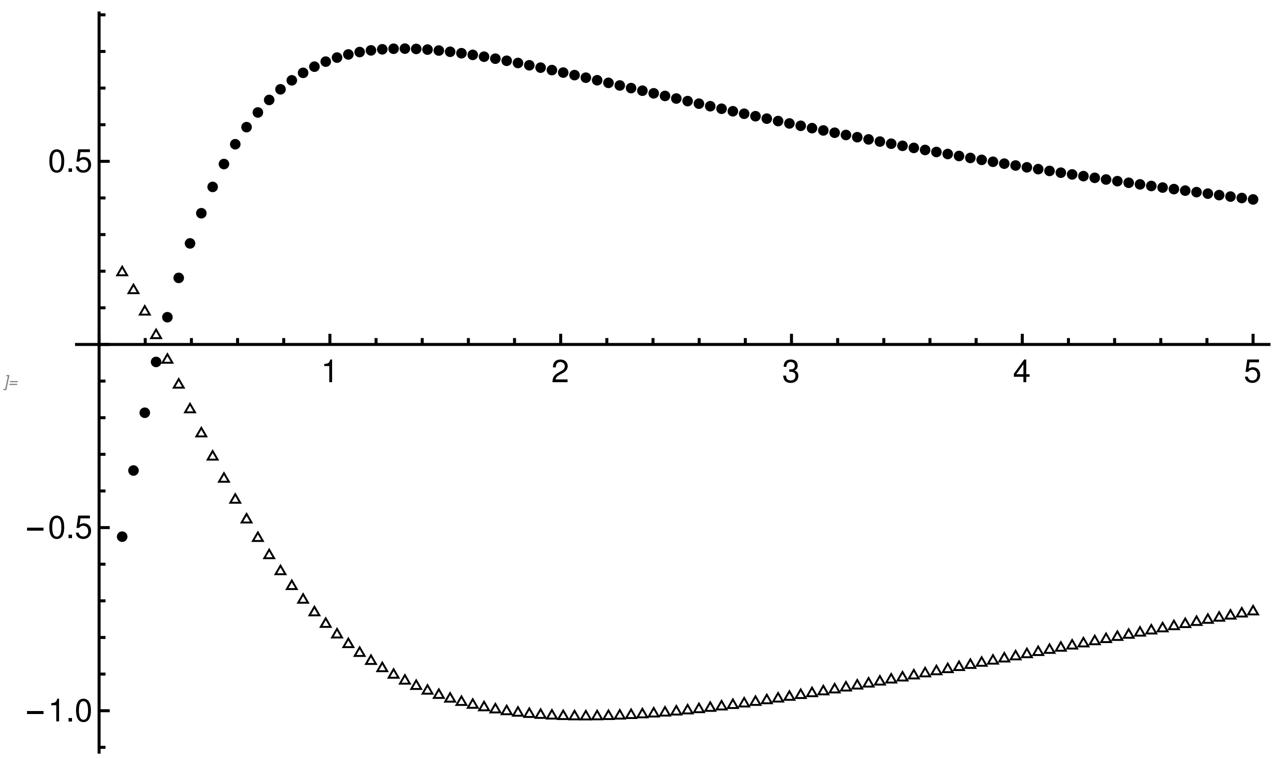
In[ ]:=
```
kB = 1.380649 × 10^-23;(*J/K*)
h = 6.62607015 × 10^-34; (*J/Hz*)
Da = 1.66053906660 × 10^-27;(*kg*)
```

```
κnum = 100;
κmin = 0.1;
κmax = 5;
Ratios4κ = Table[{}, {i, 1, κnum + 1}];
Clear[j, p, p1, p2, e, T, estar, κ, m1, m2];
For[j = 1, j ≤ κnum + 1, j++,
  κ = κmin + (j - 1) (κmax - κmin) / κnum;
  m2 = 10 Da; (*mol mass*)
  m1 = m2 / κ;  (*κ=m2/m1*)
  Tref = 300;  (*K*)
  C1 = (1/10) (m1/ρ);
  C2 = (1/10) (m2/ρ);
  a1 = 3 × 10^-49 / m1^2;
  a2 = 3 × 10^-49 / m2^2;
  ν1 = 10^-28;
  ν2 = 0.5 × 10^-28;
  (*mixture state variables*)
  ρ = 1;  (*kg/m^3*)
  u = 0 × 10^3;  (*kg m/s*)(*and hence total and interal energies are equal*)
  T = 300;
  estar = 1 / T;
  eestimate = (3/2) kB / estar (ρ / ((m1 + m2) / 2)) + (1/2) (u^2/ρ);
  numEstimate = Chop[FindRoot[FirstMEstep ∪ Projections,
     {{ρ1, ρ (0.8 - (0.6/4) κ)}, {ρ2, ρ (1 - (0.8 - (0.6/4) κ))}, {u1, u / 2}, {u2, u / 2},
      {e1, eestimate / 2}, {e2, eestimate / 2}, {ρstar, 10^3}, {ustar, 1}, {e, eestimate}}]];
  p = (-e + ρ μ + T s) /. μ → (-ρstar T) /. numEstimate;
  p1 = -e1 + ρ1 μ + T s1 /. μ → (-ρstar T) /. numEstimate;
  p2 = -e2 + ρ2 μ + T s2 /. μ → (-ρstar T) /. numEstimate;
  Ratios4κ[[j]] = {κ, ρ1 /. numEstimate, ρ2 /. numEstimate, u1 /. numEstimate,
    u2 /. numEstimate, e1 /. numEstimate, e2 /. numEstimate, p, p1, p2}];

In[ ]:= Clear[j, p, p1, p2, m1, κ, estar]
```

In[ ]:=
```
ListPlot[{Table[
   {Ratios4κ[[j, 1]], (((ρ1/ρ) (e1 + e2) - e1) - T ((ρ1/ρ) s - s1)) / ((ρ1/ρ) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
         ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
       u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
    p → Ratios4κ[[j, 8]]}, {j, 1, κnum + 1}], Table[{Ratios4κ[[j, 1]],
   (((ρ2/ρ) (e1 + e2) - e2) - T ((ρ2/ρ) s - s2)) / ((ρ2/ρ) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
         ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
       u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
    p → Ratios4κ[[j, 8]]}, {j, 1, κnum + 1}]}, AxesStyle →
  Thickness[0.0025], PlotTheme → {"Monochrome"},
 LabelStyle →
  {FontSize → 16, Black},
 AxesLabel → {Style["κ"(*"\kappa"*), FontFamily → "Times", FontSize → 20]}]
```

Out[ ]=



In[ ]:=
```
ListPlot[{Table[{Ratios4κ[[j, 1]],
    100 (p1 - (ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ1 / m1)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
       u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
     p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
   {j, 1, κnum + 1}], Table[{Ratios4κ[[j, 1]],
    100 (p2 - (ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) / ((ρ2 / m2)/(ρ1 / m1 + ρ2 / m2) p) /. m1 → m2 / Ratios4κ[[j, 1]] /.
          ρ1 → Ratios4κ[[j, 2]] /. ρ2 → Ratios4κ[[j, 3]] /. u1 → Ratios4κ[[j, 4]] /.
       u2 → Ratios4κ[[j, 5]] /. e1 → Ratios4κ[[j, 6]] /. e2 → Ratios4κ[[j, 7]] /.
     p → Ratios4κ[[j, 8]] /. p1 → Ratios4κ[[j, 9]] /. p2 → Ratios4κ[[j, 10]]},
   {j, 1, κnum + 1}]}, AxesStyle → Thickness[
   0.0025],
  PlotTheme → {"Monochrome"},
  LabelStyle →
   {FontSize → 16,
    Black}, AxesLabel →
   {Style["κ"(*"\kappa"*), FontFamily → "Times", FontSize → 20]}]
```

Out[ ]=