In[259]:=
```
"Problem 3"
Temp = 300;
Torr = 6.022 10^23 / (62.364 * Temp * 1000);
mWatt = 1.0; intensity = 1.6615 * 10^15 mWatt;
sigma = 1.078 * 10^-19;
k1 = sigma * intensity // N;
H20 = 1 Torr; x0 = 1 Torr; Argon = 760 Torr;
k2 = 3.5 * 10^-11 Exp[-2290 / Temp];
k3 = 7.8 * 10^-12 Exp[-1600 / Temp];
k4 = 1.46 * 10^-10 Exp[-593 / Temp];
k5 = 6.3 * 10^-34 Exp[900 / Temp] Argon;
tmax = 2;
Print["Cl steady state="]
Clss = Sqrt[x0 k1 / k5] / Torr
sol = NDSolve[{
   x'[t] == -k1 x[t] - k3 H[t] x[t] + k5 Cl[t] Cl[t],
   H2'[t] == -k2 Cl[t] H2[t] + k4 H[t] HCl[t],
   Cl'[t] == 2 k1 x[t] - k2 Cl[t] H2[t] + k3 H[t] x[t] + k4 H[t] HCl[t] - 2 k5 Cl[t] Cl[t],
   H'[t] == k2 Cl[t] H2[t] - k3 H[t] x[t] - k4 H[t] HCl[t],
   HCl'[t] == k2 Cl[t] H2[t] + k3 H[t] x[t] - k4 H[t] HCl[t],
   x[0] == 1 Torr, H2[0] == H20, H[0] == 0, Cl[0] == 0.00, HCl[0] == 0},
  {x, H2, Cl, H, HCl}, {t, 0, tmax}]
PageBreakAbove
Plot[Evaluate[{x[t] / Torr} /. sol],
 {t, 0, tmax}, PlotRange → All,
 AxesLabel → {"time(sec)", "Cl2(Torr)"}]
"Plot Cl and its steady state value"
Plot[Evaluate[{Cl[t] / Torr, Clss} /. sol],
 {t, 0, tmax}, PlotRange → All,
 AxesLabel → {"time(sec)", "Cl(Torr)"},
 PlotStyle → {{RGBColor[1, 0, 0]}, {RGBColor[0, 0, 1]}},
 PlotLabel → StyleForm[StyleForm["Cl", FontColor → RGBColor[1, 0, 0]] StyleForm[
     "Cl(SS)", FontColor → RGBColor[0, 0, 1]], FontSize → 12, FontWeight → "Bold"]]
"Plot H and its steady state value"
Plot[Evaluate[{H[t] / Torr,
    k2 Clss H2[t] / (k3 x[t] + k4 HCl[t])} /. sol],
 {t, 0, tmax}, PlotRange -> All,
 AxesLabel → {"time(sec)", "H(Torr)"},
 PlotStyle → {{RGBColor[1, 0, 0]}, {RGBColor[0, 0, 1]}},
 PlotLabel → StyleForm[StyleForm["H", FontColor → RGBColor[1, 0, 0]] StyleForm[
     "H(SS)", FontColor → RGBColor[0, 0, 1]], FontSize → 12, FontWeight → "Bold"]]
Plot[Evaluate[{HCl[t] / Torr} /. sol],
 {t, 0, tmax}, PlotRange → All,
```

```
 AxesLabel → {"time(sec)", "HCl(Torr)"}]
Plot[Evaluate[{H2[t] / Torr} /. sol],
 {t, 0, tmax}, PlotRange → All,
 AxesLabel → {"time(sec)", " H2(Torr)"}]
```

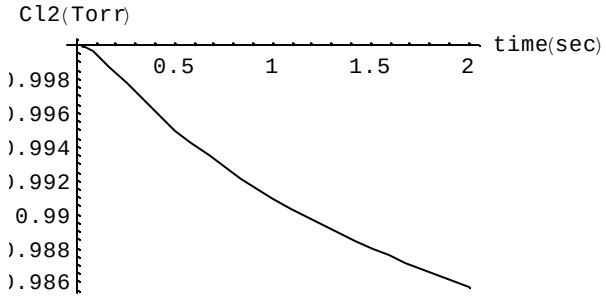
Out[259]= Problem 3

Cl steady state=

Out[272]= 0.000134077

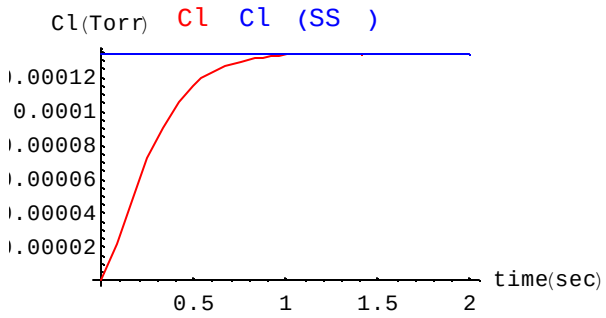
Out[273]= {{x → InterpolatingFunction[{{0., 2.}}, <>], H2 → InterpolatingFunction[{{0., 2.}}, <>],
Cl → InterpolatingFunction[{{0., 2.}}, <>], H → InterpolatingFunction[{{0., 2.}}, <>],
HCl → InterpolatingFunction[{{0., 2.}}, <>]}}

Out[274]= PageBreakAbove



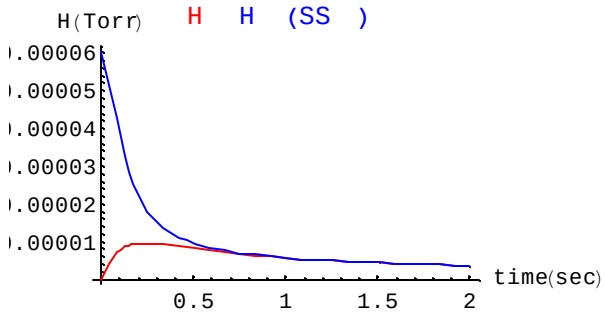
Out[275]= - Graphics -

Out[276]= Plot Cl and its steady state value

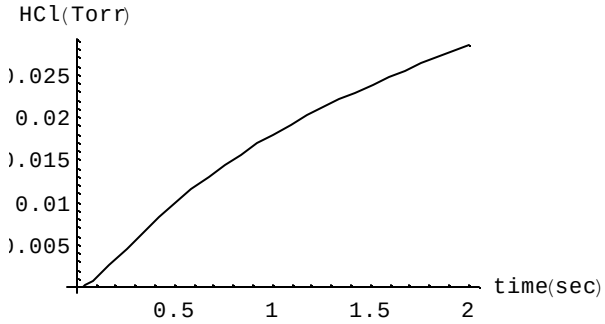


Out[277]= - Graphics -

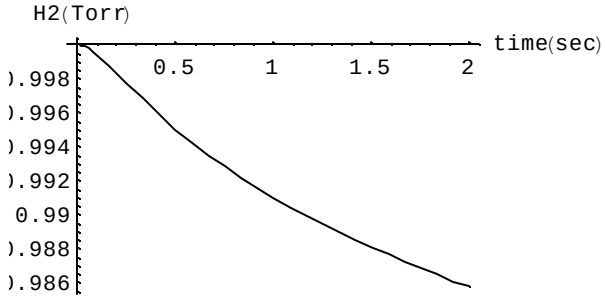
Out[278]= Plot H and its steady state value



Out[279]= - Graphics -



Out[280]= - Graphics -



Out[281]= - Graphics -