Question 1

(a) The poles of the characteristic equation of the system need to be investigated with the Routh-Hurwitz stability criterion. Specifically, the characteristic equation is:

$$1 + G(s) = 0 \Rightarrow 1 + G_c(s) \cdot G_f(s) G_p(s) G_m(s) = 0 \Rightarrow 1 + \frac{K_c \cdot 1 \cdot 0.8 \cdot (s - a)}{(s+1)(2s+1)(10s+1)} = 0$$

This can further be manipulated into:

$$1 + \frac{K_c \cdot 1 \cdot 0.8 \cdot (s - a)}{(s+1)(2s+1)(10s+1)} = 0 \Rightarrow 1 + \frac{0.8 K_c (s - a)}{20 s^3 + 32 s^2 + 13 s + 1} = 0 \Rightarrow$$

$$20 s^3 + 32 s^2 + (13 + 0.8 K_c) s + (1 - 0.8 a K_c) = 0$$

The characteristic equation has now been expanded in a polynomial form:

$$a_0 s^3 + a_1 s^2 + a_2 s + a_3 = 0 \text{, with: } a_0 = 20 \text{, } a_1 = 32 \text{, } a_2 = 13 + 0.8 K_c \text{ and } a_3 = 1 - 0.8 a K_c$$

So the Routh array can be constructed:

1	a_0	a_2
2	a_1	a_3
3	$(a_1a_2 - a_0a_3)/a_1$	0
4	a_3	

This becomes:

1	20	$13 + 0.8K_c$
2	32	$1 - 0.8\alpha K_c$
3	$\dfrac{32(13 + 0.8 K_c) - 20(1 - 0.8 a K_c)}{32}$	0
4	$1 - 0.8\alpha K_c$	

According to the Routh-Hurwitz stability criterion all coefficients of the characteristic equation need to be positive and, additionally, all elements of the first column of the Ruth array need also to be positive for the system to be stable:

- $a_0 > 0 \Rightarrow 20 > 0 \ (valid\ always)$

- $a_1 > 0 \Rightarrow 32 > 0 \ (valid\ always)$

- $a_2 > 0 \Rightarrow 13 + 0.8 K_c > 0 \Rightarrow K_c > -\dfrac{13}{0.8} \Rightarrow K_c > -16.25$

- $a_3 > 0 \Rightarrow 1 - 0.8 a K_c > 0 \Rightarrow K_c < \dfrac{1.25}{a}$

- $\dfrac{32(13 + 0.8 K_c) - 20(1 - 0.8 a K_c)}{32} > 0 \Rightarrow 32(13 + 0.8 K_c) > 20(1 - 0.8 a K_c) \Rightarrow$

  $K_c > -\dfrac{396}{25.6 + 1.6 a}$

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Considering the above and also that α is positive the stability region of the system is within the following interval:

$$\max\left\{-16.25, \quad -\frac{396}{25.6+1.6a}\right\} < K_c < \frac{1.25}{a}$$

(b) From the open-loop transfer function we see that there are three poles, so $n=3$. These poles are: $p_1=0$, $p_2=-2$ and $p_3=-4$. There is one zero, specifically $z_1=-3$, so $m=1$.

We then apply the 7 rules to construct the Root-Locus:

1. $n=3$, so the Root-Locus has three branches.

2. $m=1$, hence $n-m=2$, so there are 2 asymptotes in the Root-Locus.

3. The Root-Locus is symmetrical to the Re-axis.

4. Part of the Re-axis belongs to the Root-Locus, specifically the intervals [-4, -3] and [-2, 0].

5. The asymptotes form the following angles with the positive direction of the Re-axis:

$$\varphi_i = \frac{2k+1}{n-m}\cdot\pi, \quad k = 0,\ldots, n-m-1 \text{, hence: } \varphi_1 = \frac{\pi}{2} \text{ and } \varphi_2 = \frac{3\pi}{2}.$$

The centre of gravity of these asymptotes is:

$$\gamma = \left[\sum_{i=1}^{n} p_i - \sum_{j=1}^{m} z_i\right]\Big/(n-m) = \frac{0-2-4+3}{3-1} = -1.5$$

6. The departure/arrival points of branches can be found through the solution of:

$$\sum_{i=1}^{n}\frac{1}{(s_0-p_i)} = \sum_{j=1}^{m}\frac{1}{(s_0-z_j)} \Rightarrow \frac{1}{s_0}+\frac{1}{s_0+2}+\frac{1}{s_0+4}=\frac{1}{s_0+3} \Rightarrow$$

$$2s_0^3 + 15s_0^2 + 36s_0 + 24 = 0 \Rightarrow \begin{cases} s_{0,1} = -1.089 \\ s_{0,2} = -3.205 + 0.862i \\ s_{0,3} = -3.205 - 0.862i \end{cases}$$

Point $s_{0,1}$ belongs to the Re-axis and the Root-Locus, so it is a valid departure/arrival point. The other solutions $s_{0,2}$ and $s_{0,3}$ do not belong to the Re-axis, so they are rejected. Branches depart from the Re-axis at point $s_{0,1}$ forming an angle of ($\pm\pi/2$) with it.

7. The Root-Locus branches emanate from three simple poles and arrive at a simple zero on the Re-axis so they form 0 or π angles with its positive direction.

The final complete Root-Locus is shown below.

Root Locus

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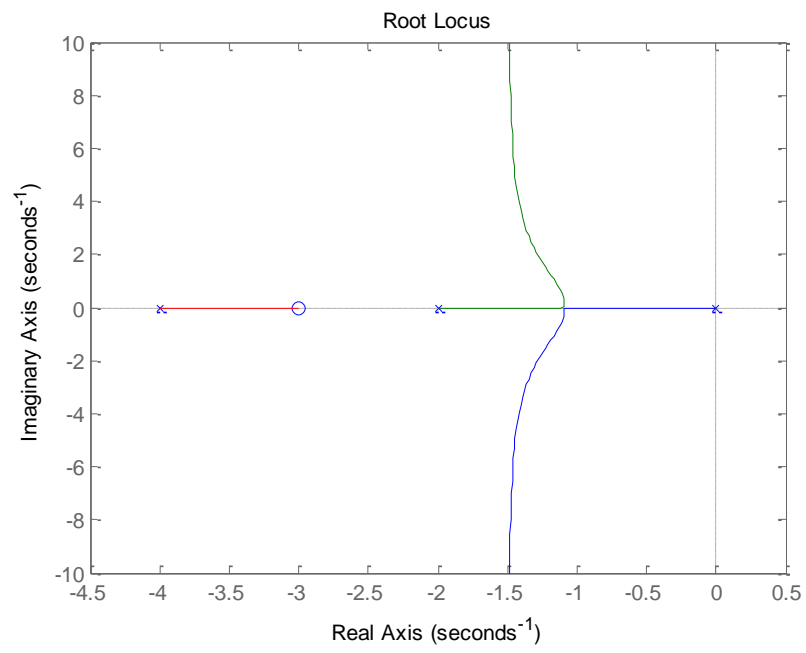
Question 2

(a) For the given transfer function, considering also that $K_p=1$, we have:

$$G(s) = \frac{1}{(100s+1)(10s+1)(s+1)} = \frac{1}{(100s+1)}\frac{1}{(10s+1)}\frac{1}{(s+1)} = G_1(s) \cdot G_2(s) \cdot G_3(s)$$

where:

$$G_1(s) = \frac{1}{100s+1}, \quad G_2(s) = \frac{1}{10s+1} \quad \text{and} \quad G_3(s) = \frac{1}{s+1}$$

Hence $G(s)$ is equivalent to three first order systems in series. For multiple systems in series, though, we know that the amplitude ratio (AR) of the overall transfer function is equal to the product of the amplitude ratios of the individual systems. As such we have:

$$AR = AR_1 \cdot AR_2 \cdot AR_3, \text{ which can be rewritten as } \log(AR) = \log(AR_1) + \log(AR_2) + \log(AR_3)$$

Also for multiple systems in series the overall phase shift is equal to the sum of the phase shifts of the individual systems, so:

$$\varphi = \varphi_1 + \varphi_2 + \varphi_3$$

For a generic first-order system with transfer function $G_x(s) = \dfrac{K_p}{\tau_p s + 1}$ the amplitude ratio is

$$AR_x = \frac{K_p}{\sqrt{1 + \tau_p^2 \omega^2}} \xrightarrow{K_p=1} \log(AR_x) = -\frac{1}{2}\log\left(1 + \tau_p^2 \omega^2\right) \text{ and the phase lag is } \varphi_x = \tan^{-1}\left(-\tau_p \omega\right),$$

so for $G(s)$ we have:

$$AR = \frac{1}{\sqrt{1 + 100^2 \omega^2}}\frac{1}{\sqrt{1 + 10^2 \omega^2}}\frac{1}{\sqrt{1 + 1^2 \omega^2}} \text{ and } \varphi = \tan^{-1}\left(-100\omega\right) + \tan^{-1}\left(-10\omega\right) + \tan^{-1}\left(-1\omega\right)$$

To create the Bode diagrams of the overall systems we need to investigate the frequency response characteristics of each system.

For $G_1(s)$:
- $\omega \to 0$: $\log(AR_1) \to 0$ or $AR_1 \to 1$. This is the low-frequency asymptote of $G_1(s)$. It is a horizontal line passing through the point $AR=1$.
- $\omega \to \infty$: $\log(AR_1) \approx -\log(100\omega)$. This is the high-frequency asymptote. It is a line with a slope of -1 passing through the point $AR=1$ for $\omega=1/100=0.01$.
- $\omega \to 0$: $\varphi_1 = \tan^{-1}(0) = 0$
- $\omega \to \infty$: $\varphi_1 = \tan^{-1}(-\infty) = -90^\circ$
- $\omega \to 0.01$: $\varphi_1 = \tan^{-1}(-1) = -45^\circ$

Similarly for $G_2(s)$:

- $\omega \to 0$: $\log(AR_2) \to 0$ or $AR_2 \to 1$. This is the low-frequency asymptote of $G_2(s)$. It is a horizontal line passing through the point $AR=1$.
- $\omega \to \infty$: $\log(AR_2) \approx -\log(10\omega)$. This is the high-frequency asymptote. It is a line with a slope of -1 passing through the point $AR=1$ for $\omega=1/10=0.1$.
- $\omega \to 0$: $\varphi_2 = \tan^{-1}(0) = 0$
- $\omega \to \infty$: $\varphi_2 = \tan^{-1}(-\infty) = -90^o$
- $\omega \to 0.1$: $\varphi_2 = \tan^{-1}(-1) = -45^o$

And for $G_3(s)$:
- $\omega \to 0$: $\log(AR_3) \to 0$ or $AR_3 \to 1$. This is the low-frequency asymptote of $G_3(s)$. It is a horizontal line passing through the point $AR=1$.
- $\omega \to \infty$: $\log(AR_3) \approx -\log(\omega)$. This is the high-frequency asymptote. It is a line with a slope of -1 passing through the point $AR=1$ for $\omega=1/1=1$.
- $\omega \to 0$: $\varphi_3 = \tan^{-1}(0) = 0$
- $\omega \to \infty$: $\varphi_3 = \tan^{-1}(-\infty) = -90^o$
- $\omega \to 1$: $\varphi_3 = \tan^{-1}(-1) = -45^o$

The resulting Bode diagrams for each individual system are shown below:
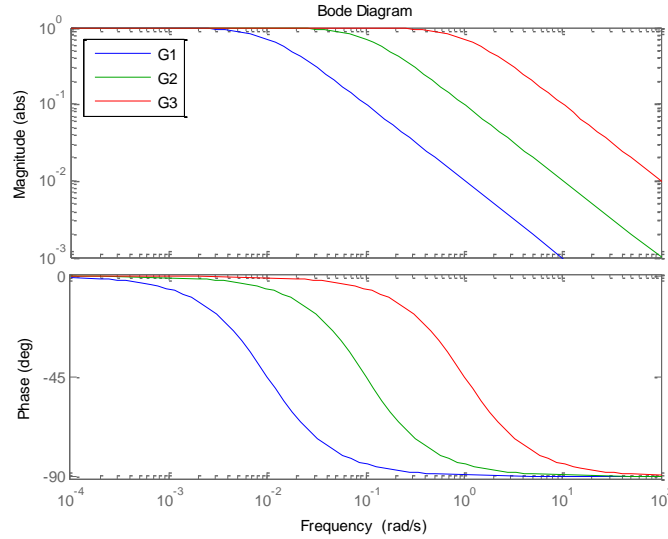
From the above we identify four distinct frequency regions. The slope of the asymptote of AR in each region is the algebraic sum of the slopes of the asymptotes for the three systems in the corresponding region. Thus we have for AR:

ω			$G_1(s)$	$G_2(s)$	$G_3(s)$	$G(s)$
0	–	0.01	0	0	0	0
0.01	–	0.1	-1	0	0	-1
0.1	–	1	-1	-1	0	-2
1	–	∞	-1	-1	-1	-3

The phase shift of the overall system will be the algebraic sum of the phase shifts of the three individual systems. A qualitative drawing can be constructed considering the values of φ_1, φ_2, and φ_3 found above at the intermediate ω values and, also, the following:

- $\omega \to 0$: $\varphi_1 \to 0$, $\varphi_2 \to 0$, $\varphi_3 \to 0$, so $\varphi \to 0$
- $\omega \to \infty$: $\varphi_1 \to -90^o$, $\varphi_2 \to -90^o$, $\varphi_3 \to -90^o$, so $\varphi \to -270^o$

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The resulting Bode diagram for the overall system is shown below:
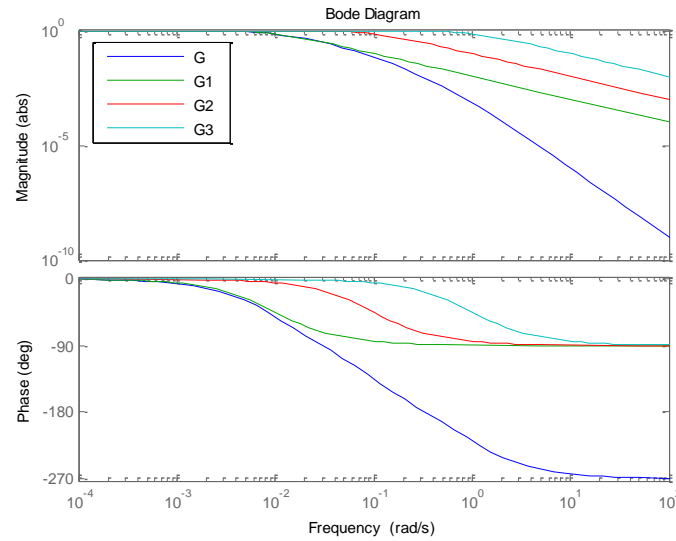
(b) The construction of the Nyquist plot is based on the corresponding Bode plot derived in (a).

- When $\omega=0$, then $AR=1$ and $\varphi=0$. Therefore, the beginning of the Nyquist plot is on the real axis where $\varphi = 0$ and at a distance from the origin $(0, 0)$ equal to 1.
- When $\omega\to\infty$, then $AR\to0$ and $\varphi \to -270°$. Therefore, the end of the Nyquist plot is at the origin where the distance from it is zero.

For every intermediate frequency $0<AR<1$ and $-270°<\varphi<0$ the Nyquist plot will be inside a unit circle and will approach the origin from the third quadrant. Its complete shape and location are shown below. A zoomed view of the approach of the plot to the origin is also shown.
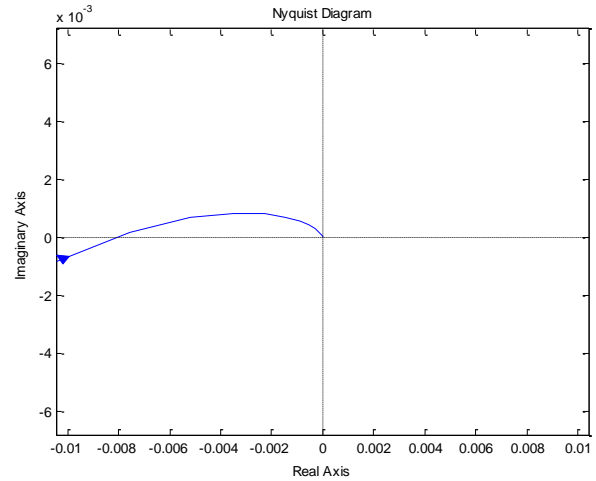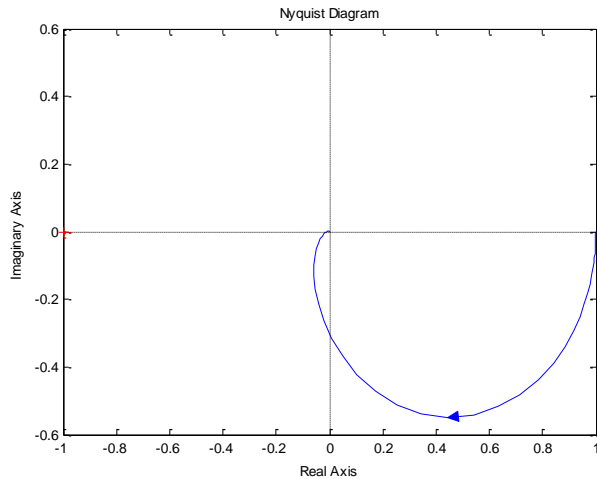
Question 3

- Use the heat in the produced water as the energy source to a Rankine cycle. Particularly the LP Separator where the water is at 90°C.
- Use the pressure in the produced water to drive a turbine coupled to an electric generator.
- The pump outlet is at 90°C – use this to pre-heat the oil from the HP Separator prior to the inter-stage heater. This will reduce the duty of the inter-stage heater and save on electrical usage.
- Instead of dropping the pressure across the HP Separator Level control valve deploy a turbine coupled to an electric generator.
- Utilise a variable speed drive on the pump to cater for reducing throughput.
- Reconfigure pumps to say 5 x 25% and progressively shut down pumps to match reducing throughput.
- Consider phased pump impeller change outs to match the declining profile.
- Utilise drag reducing agents to reduce pressure drop in pipeline.
- Install a waste heat recovery unit in GT exhaust and use heat for process.
- Convert GT to combined cycle.

Question 4:

Calculating the velocity:

$$u = \frac{Q}{\rho \times Area} = 0.5 \text{ m.s}^{-1}$$

1. We need to calculate the concentration profile at $t = 1.5$ seconds, i.e., $j = 4$. Using the finite difference scheme we can fill up the table:

	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$
$j = 1$	0.1500	1.9085	1.6570	1.0562	1.0000
$j = 2$	0.1500	1.9472	1.7494	1.0648	1.1308
$j = 3$	0.1500	1.9776	1.8547	1.0547	1.2817
$j = 4$	0.1500	1.9965	1.9778	1.0198	1.4558

2. The numerical solution at $t = 1$ second (i.e., $j = 3$) can be compared with the experimental data via $\mathcal{L}_2$ norm,)

$$\text{Norm} = \frac{||C_i^{\text{num}} - C_i^{\text{exp}}||_2}{||C_i^{\text{exp}}||_2}$$

resulting in 0.1317. The obtained norm indicates a relatively large discrepancy between numerical and experimental data.

Question 5:

1. Initial assumptions:

   - Fluids PIB, Cl·PIB·Cl, MalAnh and PIBSA are incompressible liquids with densities ρ_{PIB}, $\rho_{ClPIBCl}$, ρ_{MalAnh} and ρ_{PIBSA}, respectively. This can be lumped into a density of a liquid phase, i.e., rho_l

   - Fluids Cl_2 and H_2 are gasses with densities defined by equations of state (EOS). This can be lumped into a density of the gaseous phase ρ_g

   - Viscosities and thermal conductivities of all chemical species (lumped into phases) are known and represented by functions $\mu_j = \mu_j(T)$ and $\kappa_j = \kappa_j(T)$.

   - Geometry of the vessel, agitators and heat jackets are know and can be readily mapped;

2. Physical Formulation:

   - Fluids PIB, Cl_2 and MalAnh are added into the domain via distinct entries, whereas PIBSA, Cl_2 and H_2 are removed through two pipelines after the reaction is finished;

   - Agitator is assumed to move in a prescribed rotation (angular momentum) – $\mathcal{Q}_\Omega$;

   - The reactor is kept at a prescribed temperature through the external heat jacket;

3. Mathematical Formulation:

   - Conservative equations are given;

   - Constitutive equations:

     - fluid densities (ρ_i): equations of state

     - fluid viscosities (μ_i), thermal conductivities (κ_i) and heat capacities ($C_{p,i}$): algebraic expressions;

     - empirical and semi-empirical expressions for interphase heat transfer (γ) wall-phase heat transfer (Ω) coefficients (as function of Nu, Re and Pr dimensionless numbers);

     - differential equations representing reaction rates ($\mathcal{R}$)

   - Initial conditions: $T_i\left(\underline{x}, t=0\right)$, $P(\underline{x}, t=0)$, $\underline{u}_i\left(\underline{x}, t=0\right)$, $\alpha_i\left(\underline{x}, t=0\right)$, $\omega_{i,j}\left(\underline{x}, t=0\right)$.

   - Boundary conditions:

     - Dirichlet boundary conditions for velocity ($\underline{u}$), temperature (T_i), volume (α_i) and mass ($\omega_{i,j}$) fractions in all fluid entries;

     - No flow across the walls, baffles and agitators (Robin boundary condition):

$$\left(\frac{\partial \underline{u}_i}{\partial \underline{n}_j}\right)_{w,b,a} = 0$$

4. Pre-Processing:

   - Convert physical geometry into computational geometry (i.e., mesh generation), considering:

     - dimensionality (2- or 3-D);

     - grid shape: triangular, quadrilateral, tetrahedral, hexahedral, prismatic etc;

   - Discretisation method:

     - space (FDM, FEM, FVM, etc);

     - time (explicit, implicit or hybrid methods);

   - Solver options:

     - iterative methods;

     - direct methods as pre-conditioners;

     - tolerance;