FUNDAMENTAL CONCEPTS AND METHODS
FOR SYSTEMS MODELING
(Instructor: P.G. Georganopoulos)

PROBLEM SET # 1
Based on the Material of Lecture Units 0 and 1

0. From Lecture Unit # 0

0.1
Which of the following general principles (balance laws) governing process systems are fundamental and which are derived from others in this list? (specify what is derived from what)

1. conservation of mass
2. balance of linear momentum
3. balance of moment of linear momentum
4. balance of linear mechanical energy
5. balance of angular momentum
6. balance of angular mechanical energy
7. balance of moment of total (linear and angular) momentum
8. balance of total energy
9. balance of thermal energy
10. increase of entropy
11. balance of entropy

0.2
What type of mathematical model (macroscopic balance, maximum gradient, multiple gradient, population distribution description or macroparticle equations) do you think is adequate or most appropriate for the following process systems (we are always looking for the simplest description first but more than one levels of detail may provide acceptable answers for a given problem; however you must justify your answers):

1. unsteady-state adsorption by a fixed bed adsorber
2. chemical conversion in a plug flow reactor
3. chemical conversion in a fixed bed reactor
4. filling of an empty tank
5. steady-state two-phase flow
6. mixing and reaction in a CSTR
7. dispersion of gaseous effluent from a stack
8. distribution and metabolism of a drug or a toxicant in the human body
9. particle agglomeration
10. mass and energy transfer for a tray in a distillation column
11. a mixer with non-ideal flow patterns

0.3
How would you characterize the evolution of the following parameters of process systems with respect to (non)linearity, (non)stationarity, randomness, etc.? (more than one answer may be appropriate depending on the approximations/averaging assumptions one is willing to make; however, you must justify these assumption)

1. concentration of a heavy gas accidentally released from a chemical plant
2. ambient temperature during the month of September in Piscataway, NJ
3. fine-scale concentration of monomer in a steady-state polymerization reactor

1 From Lecture Unit # 1

1.1
Show that each of the sets of vectors

\[ e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \quad e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \ldots, \quad e_n = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix} \]

and

\[ f_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}, \quad f_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \ldots, \quad f_n = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 0 \end{bmatrix} \]

forms a basis for the real n-dimensional space of vectors \( x = [x_1, x_2, \ldots, x-n]^\top \). Find the components of \( x \) with respect to each basis.
1.2
Let \( P(n) \) be the linear vector space of all polynomials \( p = \alpha_0 + \alpha_1 t + \ldots + \alpha_n t^n \) of degree \( \leq n \) \((\alpha_i, t \in \mathbb{R})\). For arbitrary real \( t_0 \) let
\[
e_1 = 1, \quad e_2 = t - t_0, \quad e_3 = (t - t_0)^2, \quad \ldots, \quad e_{(n+1)} = (t - t_0)^n
\]
Show that \( e_1, e_2, e_3, \ldots, e_{(n+1)} \) form a basis for \( P(n) \), and find the components of an arbitrary element of \( P(n) \) with respect to this basis.

1.3
Show that the following are valid definitions of an inner product between vectors \( x \) and \( y \) in \( \mathbb{R}^2 \):
(i) \((x \cdot y) = x_1 y_1 + x_2 y_2\)
(ii) \((x \cdot y) = x_1 y_1 + \frac{1}{2} (x_1 y_2 + x_2 y_1) + 2x_2 y_2\)

1.4
For any \( f(t), g(t) \in C_{[0,1]} \) (the linear vector space of real functions that are continuous on \([0,1]\)) let the inner product be defined through \((f(t) \cdot g(t)) = \int_0^1 f(\tau) g(\tau) d\tau\). Then compute the “angle” between the functions \( \sin(k\pi t) \) and \( \sin(j\pi t) \) where \( j, k \) are positive integers.

1.5
Let \( C^*_{[0,\infty)} \) be the set of real functions defined continuous on \([0,\infty)\) and such that
\[
\int_0^\infty e^{-t} [f(t)]^2 < \infty
\]
If the scalar product in \( C^*_{[0,\infty)} \) is
\[
(f(t) \cdot g(t)) = \int_0^\infty e^{-t} f(t) g(t) dt < \infty
\]
show that \( C^*_{[0,\infty)} \) is a Euclidean space. Is it finite dimensional?

1.6
Give a detailed geometrical interpretation of the Gram-Schmidt orthonormalization process for vectors in “ordinary” 3-d space (\( \mathbb{R}^3 \)).