Course title: Computational Method in Polymeric Systems (PE4000)

Units: 3
Type: Theoretical, obligatory
Prerequisite: Null
Hours: 48

Objectives:

- Finite element method for differential equations
- Optimization of polymeric systems
- Design of experiments
- Research trends in modeling and simulation of polymeric systems

Syllabus:

Principles review:

- Macroscopic, microscopic and molecular formulation
- Formulation of differential equations based on the conservation laws
- Vectors, tensors
- Integration theory

Fundamentals of finite element and volume

- Introduction to vibrational calculus
- Finite element method for ODE: weak form, Gaussian quadrature integration, interpolation, nonlinear problems, step size analysis
- Finite element method for parabolic PDE (heat transfer, fluid flow, free surface prediction, mixing, die swell, …) including IVP ODE solution.
- Finite element method for parabolic PDE (heat transfer, polymer melt flow in die, …)
- Introduction to finite volume
- Programing in FEM using high level language such as C++, Fortran, MATLAB, …)
- Using a finite element method software such as MATLAB, COMSOL, ANSYS, Abaqus, …)

Optimization

- Basic definitions of mathematical view
- Equality and inequality constrains
- Classic optimization theory
- Numerical methods for constrained and unconstrained optimum

Design of experiments:

- Introduction to statistics: z and t distributions
- Hypothesis testing
- Experiments with a single factor (ANOVA)
- Experiments with multiple factor
- Fractional factorial methods
- Response surface method (RSM)
- Optimization based on the RSM

Research trends

- Recent researches in modeling and simulation of polymeric systems

References:

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2. E. Kreyszig, *Advanced engineering mathematics*, 10th Ed., John Wiley & Sons Inc. (2011)
3. J. N. Reddy, *An introduction to the finite element method*, 4th Ed., McGraw-Hill Inc. (2019)
4. O. Zienkiewicz, R. Taylor, and J. Z. Zhu, *The Finite Element Method: Its Basis and Fundamentals*, 7th Edition, Butterworth-Heinemann, (2013)
5. T. I. Zohdi, *A Finite Element Primer for Beginners The Basics*, Springer International Publishing, (2015)

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7. T. F. Edgar, D. M. Himmelblau, and L. S. Lasdon, *Optimization of Chemical Processes*, 2nd Ed., McGraw-Hill Book Co. (2001)
8. D. C. Montgomery, *Design and Analysis of Experiments*, 9th Ed.,John Wiley & Sons Inc. (2017)
9. R. H. Myers, D. C. Montgomery, C. M. Anderson-Cook, *Response Surface Methodology: Process and Product Optimization Using Designed Experiments,* 4th Ed., Wiley Series in Probability and Statistics, (2016)
10. Z. R. Lazic, *Design of Experiments in Chemical Engineering*, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, (2004)
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