Pandit Deendayal Energy University
School of Technology (SoT)
Department if Chemical Engineering

Minutes of Board of Studies Meeting

Date: 30-11-2021
Time: 11.00 AM – 12.30 PM
Venue: Microsoft Teams Platform
https://bit.ly/3G6D2Qn

A. Members of Board of Studies

Name of BoS Member	Name of Organization and Designation	Present / Absent	Remarks
Prof. Sameer Dalvi	IIT Gandhinagar, Professor	Present	
Prof. SS Bhagwat	ICT Mumbai, Professor	Present	
Mr. Vijay Vasudeva	Meghmani Dyes and Intermediates	Present	
Mr. NileshMangukia	Linde Group	Absent	
Miss MonideepaKarmakar	Deputy Manager, GSFC; PDEU Alumni	Present	
Mr. Ankit Pahwa	Process Design Engineer, Jacobs PDEU Alumni	Present	
Dr. Swapnil Dharaskar	Chairman, BOS Assistant Professor and HOD	Present	
Dr. Manish Kumar Sinha	PDEU, Assistant Professor	Present	
Dr. Abhishek Kumar Gupta	PDEU, Assistant Professor	Present	
Dr. Anirban Dey	PDEU, Assistant Professor	Present	
Dr. Rajesh Patel	PDEU, Dean-FOET	Present	

B. Agenda of Meeting:

(I) Open Electives:-

- **Corrosion Engineering**" from (Professional Core Elective IV) from 6thSem to be included in open elective basket in 3rd Semester.
- The open elective **Molecular Simulation** (OE-20IF201T) needs to be shifted from open elective basket floated in 4th semester to 6th Semester professional core elective basket.
- **Nanomaterials (OE-20CH205T)** subject name should be renamed as **"Introduction to Nanoscience and technology"** to appeal the response from other departments.

(II-a) Professional Core Electives: -

- **Nano Technology and Energy Storage** (20CH312T) can be shifted from **Professional Core elective basket III to Basket IV** as two expertise subject are already there in the basket III

(II-b) Proposed Elective Basket:

PCE III Basket: **Piping Design, Membrane Science and Engg**

PCE IV Basket: **Nanotechnology and Energy Storage, Environmental Engineering & Pollution Control (Proposed Subject)**, Pharmaceuticals Technology, Molecular Simulation (Shifted from Open to Core elective basket).

- New professional core elective "**Environmental Engineering & Pollution Control**" with 3 credits needs to be included in 6thsem.

(III) PhD Elective Basket:-

- The course entitled "**Molecular Modelling and Simulation**" will be introduced for Ph.D. students as it will help the student to pursue his research in the area of "computer simulations studies of complex fluids"

C. Minutes of BoS Meeting:

- **Dr. Swapnil Dharaskar, Chairman BOS** welcomed all the BOS External as well as Internal members and briefed us about the ongoing academic activities of the department as well as various initiatives taken by the department in view of the current Hybrid model of Teaching-learning pedagogy. The session then kept open for the discussion pertaining to all the agenda points

- **Agenda:** *"Corrosion Engineering" (20CH316T) needs to be shifted from PCE Basket – IV to open elective Basket of 3rd Semester.*

  Discussion: As Corrosion Engineeringis very much relevant to other engineering disciplines as well, all the BOS experts (Prof. Dalvi and Prof. Bhagwat) agreed for its inclusion as an open elective. Mr. Vasudeva however insisted of keeping the subject in 3rd year so that fundamentals and basics of other relevant subjects as well as discipline got clearer by that time. Necessary feasibility will be checked by the internal members for the possible change. **The inclusion will be effective from next academic year (AY-2022-23)**

- **Agenda:**"*Molecular Simulation" (OE-20IF201T) needs to be shifted from Open elective basket to PCE Basket- IV*

  Discussion: Molecular simulation is an important thrust area in the Chemical Engineering domain. Also, the response of this subject as an open elective is not good in recent past. So it has been decided unanimously to incorporate the subject in the departmental curriculum as a Professional Core elective (*PCE-IV*) in 6thsem. In view of this necessary changes will be framed in line with Chemical Engineering applications and included in the syllabus. Also, the Course Code needs to be relooked as the "CH" component is missing in the nomenclature.**The inclusion of the subject will be considered from next academic year (2022-2023)**

- **Agenda:** *Nanomaterials (OE-20CH205T) subject name should be renamed as "Introduction to Nanoscience and technology"*

  Discussion: In view of the generic approach of the subject as well as to gain attention from versatile engineering disciplines, the subject has been renamed and approved by all the BOS members. **The changes will be effective from next academic year (2022-23)**

- **Agenda:** "*Nanotechnology and Energy Storage" (20CH312T) needs to be shifted from PCE basket III to IV*

Discussion: As PCE basket III already consists of two expertise subjects"Piping Design", "Membrane Science and Engg" along with Laboratory components, It has been decided to shift Nanotechnology and Energy storage to PCE-IV with credit structure (3-0-0) and the lab component for this subject is omitted as most of the laboratory experiments will be taken care in other relevant subjects. **The changes will be effective from the current Academic year (2021-22).**

- **Agenda:** *New professional core elective "**Environmental Engineering & Pollution Control**" with structure (3-0-0) needs to be included in the Curriculum*

Discussion: Environmental Engineering and Pollution control play a pivotal role in the Chemical Engineering discipline. Mr. Vasudeva also suggested includingthe environmental statutory compliance portion in the syllabus of the proposed course. He also insisted that personnel from the pollution control board can take these lectures as an expert. Also, more recent case studies need to incorporate and it should be covered by Industrial experts so that students will get a practical insight into the subject.Prof. Bhagwat suggested keeping"Environmental Engineering and Pollution Control" as a core course instead of an elective. Necessary feasibility will be checked by the internal members as we need to abide by the Credit limitations. In view of this concerned subject experts from the department has been assigned the task of framing the revised syllabus taking into consideration of all the suggested changes **(Annexure-I). The changes will be effective from this current AY (2021-22)**

- **Agenda:**The course entitled "**Molecular Modelling and Simulation**" will be introduced for PhD Students

Discussion: Prof. Bhagwat and Prof. Dalvi suggested adding a tutorial/lab component in the proposed PhD course "Molecular Modelling and Simulation" to enhance the learning experience of research students. Prof. Dalvi also suggested adding crystallization as an application and thrust area in Unit-IV of the proposed PhD course (**Annexure-II**). The changes will be effective from next academic year **AY (2022-23)**

General Discussion and Recommendation by BoS Members:

- **Prof. Bhagwat** suggested changing the nomenclature of professional core elective to "**Program elective**".
- Miss. M. Karmakar (**PDEU alumni**) suggested adding Operator Tech. Simulation software such as Unisim, Prosim, etc. as a topic in relevant UG courses. Necessary inclusion can be made in the Lab component of the "Computer-aided Process Design" Subject in 7thsem.
- Mr. Ankit (**PDEU alumni**) suggested for the inclusion of relevant software-based lab components in the "**Molecular Modelling and Simulation"** subject. Also, the subject should be more application-oriented to cater to the current needs of the industry
- BOS members gave their inputs as already mentioned in detail. Internal members expressed their views and assured the external BOS members that the department will come up with necessary corrections and further improvisation recommended during the discussion.

Name of BoS Member – I Prof. Sameer Dalvi	Name of BoS Member – II Prof. SS. Bhagwat	Name of BoS Member – III Mr. Vijay Vasudeva	Name of BoS Member – IV Dr. Swapnil Dharasakr

Name of BoS Member – V Dr. Manish Kumar Sinha	Name of BoS Member – VI Dr. Abhishek Kumar Gupta	Name of BoS Member – VII Dr. Anirban Dey

Note: Take signature of all the members present in BoS

Annexure- I

Pandit Deendayal Energy University					School of Technology					
PhD Coursework					**Molecular Modelling and Simulation**					
Teaching Scheme					**Examination Scheme**					
L	**T**	**P**	**C**	**Hrs/Week**	**Theory**			**Practical**		**Total Marks**
					MS	**ES**	**IA**	**LW**	**LE/Viva**	
3	**0**	**1**	**4**	**4**	**25**	**50**	**25**	**--**	**--**	**100**

COURSE OBJECTIVES

- To introduce a range of molecular simulation techniques that are used in modelling materials and complex-fluids.
- To demonstrate the predictive capabilities of these methods by considering a set of applications.
- To able to learn efficient programming skills in accordance with the methods and algorithms of molecular modelling

UNIT 1 Introduction and overview of molecular modelling concepts

10 Hrs.

Electronic, atomic, molecular and mesoscale examples, L-J potentials, Essential principles of statistical mechanics: statistical ensembles, thermodynamic averages, fluctuations, structural quantities, time correlation functions and transport coefficients

UNIT 2 Monte Carlo simulations

10 Hrs.

Metropolis Monte-Carlo simulations, free energy calculations, CBMC Monte-Carlo, End-bridging Monte Carlo (EBMC), lattice Monte Carlo simulations, grand canonical MC simulations

UNIT 3 Molecular Dynamics Simulations

10 Hrs.

Basics of Molecular Dynamics Simulations, Numerical algorithms to solve equation of motion, Berendsen thermostat and barostat, Nose-Hoover thermostat, unconstraint and constrained dynamics, Energy minimization, canonical and microcanonical ensemble, Introduction to Brownian dynamics

UNIT 4 Applications

10 Hrs.

Polymers and polyelectrolytes in solutions, adsorption of polymers and surfactants at surfaces/interfaces, transport property calculations (diffusivity, viscosity), Applications of MC and MD techniques for– drug delivery, batteries, CO_2 sequestration Applications of MD and MD in amorphous glassy melts, MC Simulations of polymer melts and thin films,

COURSE OUTCOMES

On completion of the course, student will be able to

CO1 – **recall** and **relate** the basic concepts of molecular modelling and simulations.

CO2 – **outline** the application areas in Engineering where concept of molecular modeling can be applied.

CO3 – **choose** an appropriate molecular simulation technique and model a material or process

CO4 – **analyse**the problem statement and **compare** solutions obtained from different algorithms of MC and MD.

CO5 – estimate the properties (structure, dynamics and thermochemical) of a material or complex fluid using computer simulations.

CO6 – **formulate and solve**a real life problem statement by conducting thorough literature review of scientific literature.

TEXT/REFERENCE BOOKS

1. Leach AR, Leach AR. Molecular modelling: principles and applications. Pearson education; 2001.
2. Frenkel D, Smit B. Understanding molecular simulation: from algorithms to applications. Elsevier; 2001 Oct 19.
3. Gubbins KE, Quirke N, editors. Molecular simulation and industrial applications: methods, examples, and prospects. Taylor & Francis; 1996.

Annexure -II

Pandit Deendayal Energy University					School of Technology					
					Environmental Engineering and Pollution Control					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	3	3	25	50	25	--	--	100

COURSE OBJECTIVES

- To understand the environmental regulations and standards.
- To understand the principles and designing of air pollution control devices.
- To discuss the physical, chemical and biological characteristics of water and wastewater.
- To understand the primary, secondary and tertiary treatment process of water and wastewater.
- To learn about solid waste management and noise pollution control.

UNIT 1 – ENVIRONMENTAL STANDARDS AND AIR POLLUTION CONTROL **8 Hrs.**

Environmental regulations in India, Environmental Standards, GPCB & CPCB norms, Classification of pollutants and their permissible limits, Air pollution control: settling chamber, cyclone separators, dust collector, fabric filters, venturi scrubbers, electrostatic precipitators, wet scrubber, adsorption, absorption, Catalytic reduction eg. SCR.

UNIT 2 – PRELIMINARY AND PRIMARY TREATMENT PROCESSES **10 Hrs.**

Sources of water, Impurities in water, Indian & WHO standards for drinking water, Water borne diseases and their control, Sources of waste water, Physical, chemical and biological characteristics of water and waste water, Preliminary treatment processes: Screens, Skimming process. Primary treatment processes: Sedimentation, Coagulation and flocculation, Sand filtration.

UNIT 3 – SECONDARY AND TERTIARY TREATMENT PROCESSES **10Hrs.**

Primary treatment processes: Activated Sludge Process- design procedures for HRT, F/M ratio, SVI, MLSS, sludge age, Trickling filters and their efficiency: standard, high rate and two-stage, Sludge treatment: sludge digestion process. Tertiary Treatment Processes: Disinfection, Membrane processes, Adsorption and ion exchange, ozonation, Aeration, Softening, fluoridation, Recarbonation, Lime soda softening, Demineralization.

UNIT 4 – SOLID WASTE MANAGEMENT AND NOISE POLLUTION CONTROL **10 Hrs.**

Solid Waste Management: Quantity, Composition and characteristics of solid waste, Methods of solid waste treatment and disposal. Treatment of plastic and e-waste. Noise Pollution: level and standards, Effects and control.
Statutory Compliance, Case Studies

COURSE OUTCOMES

On completion of the course, student will be able to

CO1- **Define** environmental regulatory legislations & standards and various types of pollution.

CO2 - **Demonstrate** different types of waste generated, disposal methods, reduce and monitoring process.

CO3 - **Solve** design calculations for air pollution control devices.

CO4 - **Analyze** the properties of water and wastewater.

CO5 - **Assess** pollution control in air & noise and treatment processes of water, wastewater and solids.

CO6 - **Design** treatment units involved in water and wastewater.

TEXT/REFERENCE BOOKS

1. C. S. Rao, "Environmental Pollution Control Engineering.
2. H. S. Peavy, "Environmental Engineering", McGraw-Hill, International Ed., New York -1985