Course Name						
MODELLING AND SIMULATION OF METALLURGICAL AND MATERIALS PROCESSING						
Code	**Semester**	**Local Credits**	**ECTS Credits**	**Course Implementation, Hours/Week**		
				Theoretical	**Tutorial**	**Laboratory**
MET 346E	6	2	3	2	-	-

Department/Program	Metallurgical and Materials Engineering Department			
Course Type	Required		**Course Language**	English
Course Prerequisites	None			
Course Category by Content, %	**Basic Sciences**	**Engineering Science**	**Engineering Design**	**General Education**
		% 60	% 40	
Course Description	Introduction and fundamentals of modelling and simulation, Mathematical and physical basis of modelling, methodology, Examples of metallurgical and materials processes, Mass and energy balances, and simultaneous solutions, in-class demonstration of modelling software, Modeling and Simulation in Materials Science, Application of Multiscale Modeling, Application of the methodology for materials behavior and processing problems, Modeling of grain growth and microstructure in polycrystalline materials, Modeling of structural materials, Description of certain extractive metallurgical processes (roasting, smelting, leaching, precipitation, electrolysis, refining, etc.) and steps of their mathematical modelling, Concepts of kinetics, batch, and continuous processes in extractive metallurgy, Determining the effect of controlling parameters, such as particle size, temperature, concentration, pressure, gas/liquid/solid flow rate, stirring speed, current density, etc., and mathematical modelling thereof. Assigning these parameters to the student groups as term projects, Hands-on experimenting of modelling software in the computer-lab to investigate the effect of these parameters, individually assigned to the groups of students, Building the models of metallurgical processes, investigated under the light of related controlling parameters, their simulation with modelling software, in-class presentation of these models by the student groups to their classmates.			
Course Objectives	1. Description of metallurgical and materials processes and some simple simulation exercises, 2. Fundamentals of simulation and modelling, 3. Advances in theoretical background of metallurgical processes' simulation and modelling, 4. Demonstrating a sample commercial simulation program, 5. To have the students research on the effect of certain parameters on metallurgical processes with the help of modelling software.			
Course Learning Outcomes	Upon completion of this course, a student should be able to: 1. Understand the importance and necessity of simulation and modelling studies in metallurgical and materials processes, 2. Comprehend the data processing and process control, 3. Improve his/her theoretical background on simulation and modelling of metallurgical systems, 4. Support his/her theoretical background by hands-on application on a modelling software, 5. Be aware of the resulting innovations by applying simulation and modelling software, 6. Create a model of a given metallurgical process by considering the related control parameters.			
Textbook	R. Peter King, "Modelling and Simulation of Mineral Processing Systems", ISBN:0-7506-4884-8, 2001. Zoe H. Barber, Introduction of Materials Modeling, Maney Publishing, 2005.			
Other References	• B.A. Ogunnaike, Process Dynamics, Modelling, and Control, ISBN: 0-19-509119-1, 1994. • R.I.L. Guthrie, Engineering in Process Metallurgy, ISBN: 0-19-856367-1, 1993. • Transport and Chemical Rate Phenomena**,** N.J. Themelis, Gordon & Breach, New York, 1995. • C. Arslan, Modelling the Performance of Aqueous Chromium Electrowinning Cells, Ph.D. Thesis, Columbia University, New York, 1991. • E. Peters, D. Dreisinger, Mixing, Leaching and Modelling Course Notes, Metals and Materials Eng. Dept. Univ. of British Columbia, Vancouver, Canada, 1990. • R.G. Bautista, R.J. Wesely, G.W. Warren, Hydrometallurgical Reactor Design and Kinetics, A Publication of The Metallurgical Society, Inc., U.S.A., 1986. • A.W. Bryson, Modelling the Performance of Electrowinning Cells, Proceedings Hydrometallurgy 81, Manchester 1981, pp.G2/1-G2/11, 1981. • Dierk Raabe, Computational Materials Science, Wiley VCH Verlag GmbH, 1998. • Z. Xiao Guo (Ed), Multiscale Materials Modelling: Fundamental and Applications. Woodhead Publishing Limited, Cambridge, 2007.			
Homework & Projects				
Laboratory Work				
Computer Use	Within the context of this course, each student group is assigned with a metallurgical process and is expected to model that process through the semester with the help of commercial software (CadsimPlus or IDEAS). At the end of the semester they will present their model in front of their classmates.			
Other Activities				

Assessment Criteria		**Quantity**	**Effects on Grading, %**
	Activities	-	-
	Midterm Exams	1	35 %
	Quizzes	-	-
	Homework	-	-
	Projects	-	-
	Term Paper/Project	1	15 %
	Laboratory Work	-	-
	Other Activities	-	-
	Final Exam	1	50 %

COURSE PLAN

Weeks	Topics	Course Outcomes
1	Fundamentals of modelling and simulation, Mathematical and physical basis of modelling, methodology,	1, 2
2	Examples of metallurgical and materials processes, simultaneous solutions.	1, 2
3	Examples of metallurgical and materials processes, Mass and energy balances, and simultaneous solutions.	1-4
4	Fundamentals of modelling and simulation, in-class demonstration of modelling software.	1-4
5	Simulation methods of materials science, Application of the methodology for materials behavior and processing problems,	2, 3
6	Modeling of grain growth and microstructure in polycrystalline materials, Modeling of structural materials,	2, 3
7	Description of certain extractive metallurgical processes (roasting, smelting, leaching, precipitation, electrolysis, refining, etc.) and steps of their mathematical modelling.	2, 3
8	Concepts of kinetics, batch, and continuous processes in extractive metallurgy.	1-3
9	Determining the effect of controlling parameters, such as particle size, temperature, concentration, pressure, gas/liquid/solid flow rate, stirring speed, current density, etc., and mathematical modelling thereof. Assigning these parameters to the student groups as term projects.	4-6
10	Hands-on experimenting of modelling software in the computer-lab to investigate the effect of these parameters, individually assigned to the groups of students.	4-6
11	Hands-on experimenting of modelling software in the computer-lab to investigate the effect of these parameters, individually assigned to the groups of students.	4-6
12	Building the models of metallurgical processes, investigated under the light of related controlling parameters, their simulation with modelling software, in-class presentation of these models by the student groups to their classmates.	4-6
13	Building the models of metallurgical processes, investigated under the light of related controlling parameters, their simulation with modelling software, in-class presentation of these models by the student groups to their classmates.	4-6
14	Building the models of metallurgical processes, investigated under the light of related controlling parameters, their simulation with modelling software, in-class presentation of these models by the student groups to their classmates.	4-6

Relationship between the Course and Metallurgical & Materials Engineering Curriculum

	Program Outcomes	Level of Contribution		
		1	2	3
1	Ability to apply the knowledge of mathematics, science, and engineering principles to solve problems in metallurgical and materials engineering (ABET:a)			X
2	Ability to characterize materials using standard and/or self designed experimental methods and to evaluate the results (ABET:b)	X		
3	Ability to design a system or a process, taking into consideration of the desired specifications, quality, ethics and environment (ABET:c)			
4	Ability to communicate both orally and in the written form and to take part in, and provide leadership of the teams in the elucidation of engineering problems (ABET:d, g)			
5	Ability to define, formulate and solve engineering problems in the development, production, processing, protection and usage of engineering materials (ABET:e)			X
6	An understanding of professional and ethical responsibilities (ABET:f)			
7	An understanding of current/contemporary issues and impact of engineering solutions in broad cultural, national and global levels (ABET:h, j)		X	
8	A comprehension of the nature of engineering progress closely linked with the development of new materials and production processes. An ability to engage in life-long learning and a recognition of its necessity (ABET:i)		X	
9	Ability to use essential tools and techniques of modern engineering in the development, production, processing, protecting of the existing and new engineering materials (ABET:k)			X

1: Little, 2: Partial, 3: Full

Course relationships with major elements of the field and material classes

		Level of Contribution		
		1	2	3
MAJOR ELEMENT OF THE FIELDS	**STRUCTURE**		X	
	PROPERTIES			X
	DESIGN EXPERIMENT/ANALYSE DATA			X
	PROCESSING			X
	COST/PERFORMANCE		X	
	QUALITY/ENVIRONMENT		X	
	DESIGN PROCESS OR PRODUCT			X
MATERIAL CLASSES	**METAL**			X
	CERAMICS			
	POLYMERS			
	COMPOSITES			

1: Little, 2: Partial, 3: Full

Prepared by	**Date**	**Signature**
Prof. Dr. Cüneyt ARSLAN Prof. Dr. Sebahattin GÜRMEN	December 2020	