Simulation practice with Modelica

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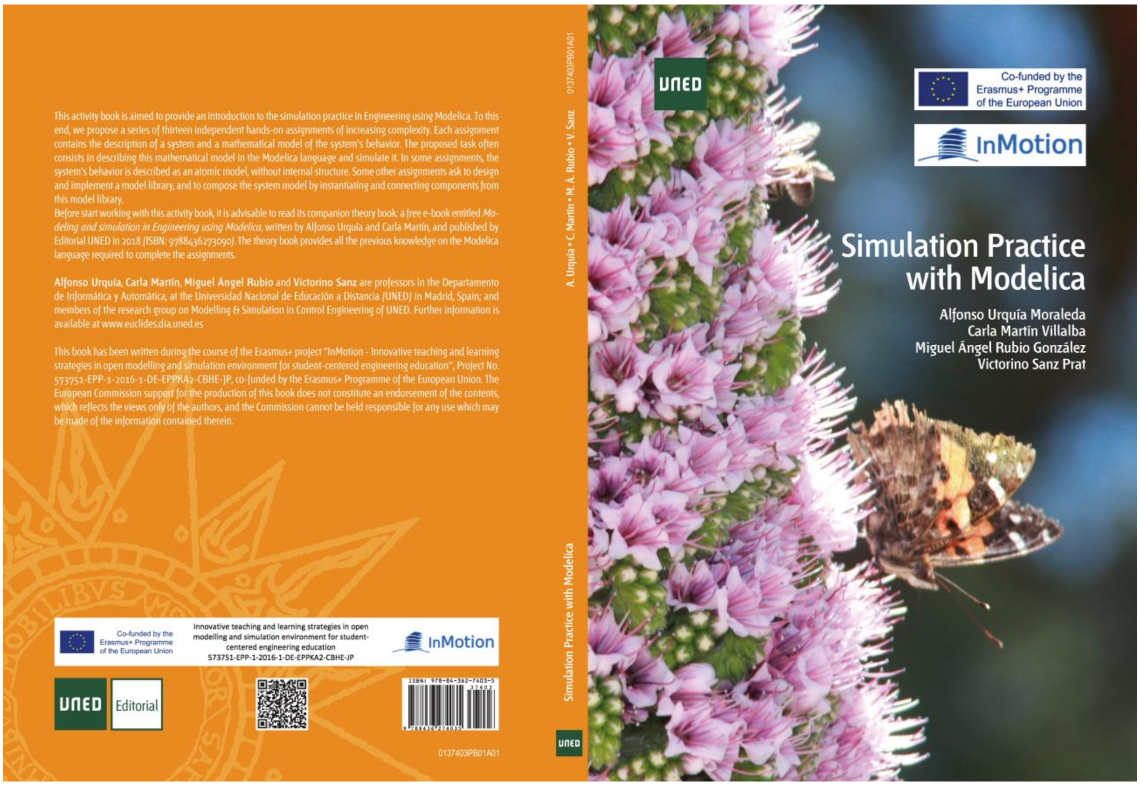
Activity book abstract



This activity book consists of thirteen assignments that have been specifically designed to practice the concepts explained in the theory companion book, entitled "Modeling and simulation in Engineering using Modelica". The **target audience** are bachelor's or master's level students, interested in modeling and simulation, and with a background in both physics and numerical methods.

The learning objectives of the assignments are summarized in Table 1, which is placed at the end of this document. Some assignments contain system descriptions and students are asked to write the corresponding mathematical models. This allows students to practice mathematical modeling in the mechanical and thermo-hydraulic domains. In assignments dealing with models of greater complexity, such as the heat exchanger, "The Game of Life" cellular automaton, the transport of atmospheric pollutants, the simplified Tennessee Eastman process, and the fuel cell, the mathematical models are discussed in the assignment descriptions.

Students are asked to describe in Modelica the mathematical models of the systems and simulate them. An atomic description of the model is required in some cases. In other cases, the task consists in decompose the system model into parts, design and implement a Modelica library containing models of the system parts, and finally compose the system by instantiating and connecting components from the library.

Additionally, students are asked to perform analyses on the model, such as to calculate the model computational causality and pose its initialization problem; to design experiments, run the corresponding simulations and draw conclusions; to analyze the simulation performance; and to implement graphical animations for the simulations.

The co-simulation of Modelica models with external simulation code is also practiced. The assignment on the cellular automaton known as "The Game of Life" allows students to experience with the external function interface of Modelica. The assignment on the simplified Tennessee Eastman process includes embedding a Modelica model into a Simulink block using FMI.

A brief description of the assignments' topics and the instructions for students is provided next.

A mechanical system composed of two springs, a damper, a pulley and a lever is described in **Assignment 1**. Students are asked to write the system dynamical model, analyze its computational causality, write by hand its simulation algorithm, describe the model in Modelica as an atomic model, employ the information generated during the model translation to check whether their computational causality analysis is correct, and run the simulation.

Another mechanical system is described in **Assignment 2**. The system is composed of two springs, a pulley and a hanging load. Students are firstly asked to write the system dynamical model; then, to pose and solve by hand the initialization problem for three different sets of initial conditions; and finally, to describe the model in Modelica as an atomic model, simulate it for the three different sets of initial conditions, and to compare the solutions they have calculated by hand with the simulation results.

Students are introduced to the bond graph modeling methodology in **Assignment 3**. To this end, they are firstly asked to read a clear and concise introduction to the bond graph modeling methodology. Next, students are asked to write the bond graph models of three mechanical systems, and to perform the causal analyses. Finally, students are asked to develop a Modelica library containing bond graph elements and, using this library, to compose the Modelica models of the three mechanical systems.

The characteristic curve of a liquid source is graphically described in **Assignment 4**. According to this curve, the actual mass flow rate provided by the source depends on the set-point value, and also depends on the load pressure, this is, the pressure exerted by the environment at the source-to-environment connection point. As it is described in the assignment, the liquid source is a simple example of variable structure model, well-suited for practicing the use of Modelica if expressions and clauses. Students are asked to program a Modelica library containing the source model class, and several record classes specifying particular parameter values.

The model of a heated ideal gas is employed in **Assignment 5** to reinforce understanding on how variable structure models are described in Modelica. The mathematical model of the system is given, and the proposed task consists in describing it in Modelica, setting its initial conditions and simulate it.

Assignment 6 is aimed for practicing modeling of finite-state machines in Modelica. The system at hand is a closed control loop, composed of the connection of a single-input single-output plant and a hysteresis controller. The characteristic curve of the controller is provided. The plant is described by a set of first-order, linear, ordinary differential equations. Firstly, students are asked to describe the controller behavior as a finite-state machine, which has four modes. Next, students are asked to develop a Modelica library containing the controller, the plant and the complete system. In doing this, the following specifications have to be satisfied: the controller and plant have to be described as Modelica block classes, and the dimension of the plant's state has to be a parameter.

The filling and draining dynamics of a tank used to store benzene is analyzed in **Assignment 7**. The tank is drained through a horizontal circular pipe, connected at one end to the tank bottom, and at the other end to an atmospheric pressure sink. The balance of linear momentum is applied to the benzene that flows through the pipe, taking into account the friction force exerted by the pipe wall. The operation of the plant composed of the benzene source, the tank, the pipe and the sink is simulated. To this end, students are asked to develop a Modelica library.

The system modeled in **Assignment 8** is composed of two liquid storage tanks connected through a pump. A liquid source, connected to the first tank, can pump a mixture of kerosene and benzene into the tank, or drain the tank content. The second tank is heated. The two tanks are modeled as closed vessels, implying that the volume of liquid stored within a tank cannot be greater than the tank volume. The set-point signals of the source, pump and heater are generated by three controllers that describe the following operation steps: (1) the source introduces the liquid mixture into the first tank; (2) the pump transfers liquid from the first tank to the second one during a certain time; (3) the liquid stored in the second tank in heated; (4) the pump transfers the content of the second tank to the first one; and (5) the liquid source drains the first tank. Students are asked to write the system mathematical model, design and develop a Modelica library, use it to compose the system model and simulate it.

The system modeled in **Assignment 9** is a double-pipe heat exchanger employed to cool down a gas mixture using water as coolant. The values of the relevant physical parameters, and the equations to calculate the heat transfer coefficients, are given.

Students are asked to perform a spatial discretization of the gas and water streams, and the inner pipe wall, and to write the steady-state energy balances in the obtained control volumes. Next, students are asked to describe the heat exchanger in Modelica as an atomic model, and to experiment with it by running a certain experimental design.

The cellular automaton known as "The Game of Life" is modeled in **Assignment 10**. The Game of Life is a two-dimensional cellular automaton proposed by John H. Conway in 1970, with the purpose of studying the evolution of the different patterns that arise from different initial configurations of the cellular space. The rules that define the evolution of the cellular automaton are explained in the assignment. Firstly, students are asked to write a Modelica model that evolves according to these rules, and generates a graphical animation displaying the automaton evolution. Then, they are asked to evaluate the maximum size of cellular space that can be simulated using their model. Next, students are asked to replace the Modelica description of the automaton behavior by a description in the C programming language, using also external libraries such as gnuplot to implement the graphical animation. Finally, students are asked to compare the two implementations in terms of size of the cellular space and execution time.

The transport and dispersion into the atmosphere of the pollutants emitted by an industrial chimney is simulated in **Assignment 11**. The effect on the plume shape of the meteorological conditions, the terrain, and the emission factors is described using a Gaussian plume model that is discussed in the assignment. Students are asked to develop a Modelica model to calculate the pollutant concentrations as a function of the spatial position.

The Tennessee Eastman model is a well-known benchmark that describes a real industrial chemical process. The model considered in **Assignment 12** is a simplified variant of the Tennessee Eastman model. The assignment contains a description of the simplified Tennessee Eastman model, and three tasks. Firstly, students are asked to develop a Modelica library for describing the simplified Tennessee Eastman model. Secondly, students are asked to model an automatic control strategy, by using the Simulink block diagram environment. Finally, students are asked to export the Modelica model as a Functional Mockup Unit and embed it into a Simulink block, developing the closed-loop system model in Simulink.

Modeling of proton exchange membrane fuel cells is addressed in **Assignment 13**. The assignment contains a didactic introduction to the fuel cell structure, and the most relevant physical-chemical phenomena that take place in the fuel cell cathode, including the following: transport of liquid-phase and gas-phase water in the diffusion layer and the active layer; transport of oxygen in the diffusion layer and the active layer; electrical conduction in the active layer and the diffusion layer; proton conduction in the membrane and the active layer; and electrochemical reaction in the active layer. The student's work is structured in Assignment 13 into three tasks.

Task 1 consists in developing a one-dimensional Modelica model of gas diffusion in a porous material, to calculate the gas pressure and molar flow rate as a function of the spatial coordinate and time.

The objective of Task 2 is to extend the Modelica model developed in Task 1, by considering a second gaseous species and the liquid phase. The modeled phenomena are the diffusion of oxygen, steam water and liquid water in a porous medium; and the balance of steam water and liquid water due to evaporation and condensation processes.

Students are asked in Task 3 to model in Modelica the electric conduction, and electrochemical reaction. The objective is twofold. Firstly, to model the electron and proton conduction in the membrane, the catalyst layer and the diffusion layer of the cathode. Secondly, to model the electrochemical reaction that takes place in the catalyst layer. Combining these models with the models developed in the previous two tasks, the complete model of the PEM fuel cell is obtained. Finally, students are asked to describe the electrical circuit required to polarize the PEMFC model, and to perform a series of simulations to obtain the polarization curves of the fuel cell.

Table 1: Assignments and learning objectives

Assignment	**Learning objectives**
1. Springs, damper and lever	– Practice modeling of simple mechanical systems composed of springs, dampers and levers. – Analyze the computational causality of DAE systems. – Describe a DAE system as an atomic model in Modelica, and simulate the model.
2. Springs, pulley and load	– Practice modeling of simple mechanical systems composed of springs, pulleys and loads. – Describe a DAE system as an atomic model in Modelica, setting the initial conditions.
3. Bond graph library	– Getting started with bond graph modeling using Modelica. – Design and implement model libraries in Modelica.
4. Source of liquid	– Use if expressions, if clauses, and records.
5. Ideal gas in a heated container	– Practice modeling of variable structure systems. – Practice the use of the unit, start and fixed attributes.
6. Hysteresis controller	– Practice modeling of finite state machines. – Practice the declaration and use of block classes, and matrix equations.
7. Draining of a benzene storage tank	– Practice developing a library, and composing a model by instantiating and connecting library components.
8. Heating a liquid mixture	– Practice modeling of simple thermo-hydraulic systems, posing mass and energy balances, and describing changes in the liquid flow direction. – Describe multi-mode models in Modelica.
9. Double-pipe heat exchanger	– Practice modeling of cocurrent and countercurrent heat exchangers, with local variations in physical properties and heat transfer coefficients. – Use array variables in Modelica. – Facilitate the numerical solution of models with systems of simultaneous nonlinear equations.
10. Cellular Automata -- The Game of Life	– Modeling and simulation of discrete-event models using Modelica. – Experience and practice with the external function interface of Modelica. – Implement graphical animations for the simulations using visualizers of the Modelica.Mechanics.Multibody library, and gnuplot. – Analyze the simulation performance.
11. Air pollution	– Get insight into the Gaussian plume model. – Use arrays, for loops, and enumeration types. – Describe a DAE system as an atomic model in Modelica.
12. Simplified Tennessee Eastman model	– Practice modeling of hydraulic components and simple chemical reactors. – Use records to describe fluid properties. – Use arrays of variables and for loops. – Embed a Modelica model into a Simulink block using FMI.

13. PEM fuel cell	– Practice modeling PEM fuel cells, which implies modeling gas and liquid diffusion in porous media, electrochemical reactions, and electric circuits. – Use spatial discretization to solve partial differential equations (PDE) in Modelica.

The activity book written by Alfonso Urquía, Carla Martín, Miguel Ángel Rubio and Victorino Sanz (UNED).

Editorial UNED (Madrid, Spain), 2018, ISBN 978-84-362-7403-5