Lecture#6: **Basic Functions of COMSOL Multiphysics**

Goal

This lecture introduces students to the fundamental principles and workflow of COMSOL Multiphysics, a finite-element-based simulation environment used for solving multiphysics problems. Students will learn how to construct geometries, assign physics interfaces, generate meshes, define studies, and visualize results. Special emphasis is placed on its application in electrochemical modeling, particularly copper electrodeposition, demonstrating how COMSOL integrates transport, potential, and kinetic processes into a unified simulation framework.

COMSOL Multiphysics is a comprehensive software platform designed to solve multiphysics problems by combining different physical models. It is widely used in fields such as engineering, physics, and materials science for simulating various phenomena like heat transfer, structural mechanics, fluid dynamics, and electromagnetism. Here, we will explore the “basic functions” of COMSOL and how it can be applied for solving real-world problems.

1. Introduction to COMSOL Multiphysics

COMSOL is a finite element analysis (FEA) tool that provides an integrated environment for modeling and simulating coupled physical systems. It allows users to define geometries, set up physical models, solve partial differential equations (PDEs), and visualize results.

Key Features:

- Multiphysics Simulations: COMSOL allows simultaneous simulation of different physical phenomena, such as fluid flow coupled with heat transfer, or electromagnetic fields with structural mechanics.

- User-friendly Interface: It provides a graphical interface for defining and solving problems without needing to write code, although scripting in COMSOL’s Java-based API is also possible.

- Customization and Extensibility: Users can create custom physics interfaces and couple them with the built-in physics models.

2. Basic Workflow in COMSOL Multiphysics

The basic workflow for setting up and solving a problem in COMSOL involves the following steps:

Step 1: **Defining the Geometry**

The first step is creating or importing the geometry of the model. COMSOL offers built-in geometry tools that allow users to draw 2D or 3D shapes and use operations like union, subtraction, and intersection.

- CAD Import Module: Enables importing geometries from popular CAD software formats.

- Geometry Node: All geometries are created and modified here.

Step 2: **Assigning the Physics**

COMSOL provides a large library of predefined “physics modules”, including heat transfer, fluid flow, electromagnetics, and structural mechanics. These modules are customizable and can be used to simulate real-world scenarios.

- “Physics Interface": Choose appropriate physics for the problem (e.g., “Heat Transfer in Solids”, “Laminar Flow”, or “Electrostatics”).

- “Multiphysics Coupling”: Easily couple multiple physics modules. For example, combining “Fluid Flow” and “Heat Transfer” for simulating convective cooling.

Step 3: **Meshing**

Meshing involves discretizing the geometry into smaller elements (finite elements) for numerical computation. COMSOL provides automatic and manual meshing options, which allow you to control the density of the mesh for accuracy and efficiency.

- Free Tetrahedral Mesh: Commonly used for 3D geometries.

- Adaptive Meshing: Automatically refines the mesh based on error estimates.

Step 4: **Defining Study and Solving**

Once the geometry, physics, and mesh are defined, the next step is setting up the “study”. A study defines how the simulation is run, including the type of solver used (e.g., time-dependent or stationary), and the boundary and initial conditions.

- Study Types: COMSOL supports stationary, time-dependent, eigenvalue, parametric, and frequency-domain studies.

- Solvers: The software has robust solvers, such as direct solvers (e.g., MUMPS) and iterative solvers (e.g., GMRES), to handle complex and large-scale simulations.

Step 5: **Post-Processing and Visualization**

Once the solution is obtained, COMSOL provides powerful visualization tools for analyzing results. You can generate plots such as “surface plots”, “line graphs”, “streamlines”, and “contour plots”.

- “Post-Processing Tools”: These allow you to visualize physical quantities (e.g., temperature, electric field, velocity) over the model’s geometry.

- “Export Options”: Results can be exported in different formats for further analysis.

3. Key Physics Interfaces in COMSOL

COMSOL offers a range of physics interfaces, organized by domain:

i. Heat Transfer Module:

- Models heat conduction, convection, and radiation.

- Can be coupled with other modules for onjugate heat transfer problems, where heat transfer and fluid flow are coupled.

ii. Fluid Flow Module:

- Simulates laminar and turbulent flow in 2D or 3D.

- Applicable in engineering problems such as flow through pipes, aerodynamics, and fluid-structure interaction (FSI).

iii. Chemical Engineering Module:

- Models mass transport, reaction kinetics, and chemical species diffusion.

- Can simulate processes like corrosion, battery performance, and chemical reactors.

4. Multiphysics Coupling and Customization

One of COMSOL’s strengths is its ability to couple different physics to solve complex, real-world problems. For example:

- Electrochemical Deposition: Coupling electrostatics with mass transport for modeling deposition rates in electroplating.

- Thermo-Fluid Systems: Coupling fluid flow with heat transfer to model convective heat transfer in electronics cooling.

5. COMSOL Interfaces and Tools

COMSOL Application Builder:

- Allows users to create custom simulation applications with simplified user interfaces, ideal for non-experts.

COMSOL Server:

- Enables sharing and running of COMSOL applications over a network or the internet, which is useful in collaborative environments or for deployment purposes.

Example: Copper Electrochemical Deposition in COMSOL

Consider the example of modeling *copper electrochemical deposition* in an electrolyte. In this case, the physics would involve:

- Electrostatics: For modeling the electric potential distribution.

- Transport of Diluted Species: To account for the movement of copper ions (Cu^{2+}) towards the electrode.

- Butler-Volmer kinetics: For modeling the electrode reaction.

Steps in COMSOL:

1. Define Geometry: Set up the cathode, electrolyte, and anode geometries.

2. Assign Physics: Select Electrostatics and Transport of Diluted Species. Define reaction kinetics using the Butler-Volmer equation.

3. Meshing: Create a fine mesh near the electrode for higher accuracy.

4. Solving: Perform a time-dependent study to simulate the deposition over time.

5. Post-Processing: Visualize the concentration of Cu^{2+} ions and deposition thickness.

Advantages of COMSOL Multiphysics

- Flexible Multiphysics Coupling: Allows seamless integration of different physics, which is vital for solving real-world problems.

- Extensive Physics Library: COMSOL covers a wide range of domains, making it versatile for multidisciplinary applications.

- Intuitive Interface: Provides a balance between ease of use and functionality, which is useful for both beginners and experts.

- High-Performance Solvers: Efficient solvers can handle large-scale simulations and complex systems.

Learning Outcomes

By the end of this lecture, students will be able to:

1. Explain the basic concepts of finite-element analysis (FEA) and its implementation in COMSOL Multiphysics (related to LO 4, ID 4.1).

2. Navigate the COMSOL interface and identify major components: geometry, physics, mesh, study, and results modules (related to LO 4, ID 4.2).

3. Apply core workflow steps for building and solving a COMSOL model, including geometry creation, meshing, solver setup, and visualization (related to LO 4, ID 4.2–4.4).

4. Select and configure physics interfaces relevant to chemical-engineering and electrochemical systems—such as Electrostatics and Transport of Diluted Species (related to LO 4, ID 4.3–4.5).

Questions and Self-Study Assignments

1. What is finite-element analysis (FEA), and how does COMSOL Multiphysics implement it?

2. List and briefly describe the five core steps in the COMSOL modeling workflow.

3. Compare automatic vs. manual meshing and explain when each should be used.

4. What is the function of a physics interface in COMSOL? Provide three examples relevant to chemical engineering.

5. Explain how multiphysics coupling works in COMSOL using an example (e.g., coupling heat transfer and fluid flow).

6. Describe how the Butler–Volmer equation can be implemented within COMSOL to model electrode kinetics.

7. Identify and explain the roles of solvers (direct and iterative) in numerical simulations.

8. Design a simple COMSOL study for copper electrodeposition: outline geometry, physics, boundary conditions, and expected outputs.

9. (Optional) Read one recent paper (published within the last 3 years) employing COMSOL for electrochemical modeling. Summarize:

- type of process modeled;

- physics interfaces used;

- main conclusions regarding process optimization or deposition uniformity.

References

1. Finlayson B.A. Introduction to Chemical Engineering Computing. Second Edition. - John Wiley & Sons, 2012., DOI: 10.1002/9781118309599

2. Pryor R.W. Multiphysics Modeling Using COMSOL5 and MATLAB. - Mercury Learning and Information, 2015. – 700 p.