Screening Task: Chemical Process Simulation Library Development in OpenModelica

STAGE 1: SCREENING TASK SUBMISSION: Complete the screening task as described below:

This screening assignment is intended to identify fellows capable of contributing to the development of a chemical process simulation library using OpenModelica. The screening emphasizes equation-based modeling skills, chemical engineering fundamentals, and library-oriented design thinking.

General Instructions

- Use OpenModelica (latest official release version recommended).
- External commercial simulators (e.g., DWSIM, Aspen, HYSYS, gPROMS) must not be used.
- All models must be written using equation-based modeling.
- Use SI units via Modelica.Units.SI.
- Submit Modelica source files and a short technical note (2–3 pages).

Important: Completion of Step 1 and Step 2 is mandatory to be considered for the internship. Step 3 is optional and will be used to identify top-performing candidates.

Step 1 (Mandatory): Steady-State CSTR Model

Objective: Develop a reusable steady-state Continuous Stirred Tank Reactor (CSTR) model in OpenModelica.

Process Description:

A single irreversible reaction occurs in a perfectly mixed, isothermal CSTR:
$A \rightarrow B$

Reaction rate (first order): $r_A = k C_A$
Assume constant density and steady-state operation.

Model Inputs:

- Feed volumetric flow rate (F)
- Feed concentration of A (CA_in)
- Reactor volume (V)
- Reaction rate constant (k)

Model Outputs:

- Outlet concentration of A (CA_out)

- Conversion of A (X)

Mandatory Modeling Requirements:

- Use Modelica connectors for material flow
- Formulate balances using equation sections only
- Avoid hard-coded numerical values inside equations
- Model must be modular and reusable

Step 2 (Mandatory): Library-Oriented Reactor Design

Objective: Refactor the reactor model into a reusable unit-operation suitable for inclusion in a chemical process simulation library.

Requirements:

- Create a partial base reactor model (e.g., BaseReactor)
- Do not hard-code reaction kinetics in the base model
- Implement reaction kinetics using a replaceable model (e.g., FirstOrderReaction)
- Demonstrate one concrete reactor extension (CSTR, Batch Reactor, or simple PFR)

Step 3 (Optional): Property and Kinetics Extension

Objective: Demonstrate advanced capability to extend the library with supporting physical models.

Choose one or both of the following:

- Implement a simple ideal-liquid density model
- Implement a temperature-dependent Arrhenius reaction rate model

Submission Guidelines

- Submit all Modelica (.mo) files in a single compressed folder.
- Include a short technical note explaining assumptions, model structure, and usage.
- Clearly document any limitations or simplifications.
- Upload the compressed folder in the g-drive and submit the link of g-drive in this form: https://forms.gle/WbkWVYgvhXXWJ94D7

STAGE 2: PERSONAL INTERVIEW ROUND: Candidates will be shortlisted based on the screening task, and selected candidates may be invited for an interview before the final selection is announced.