Proposal for announcing seat under the Institute Internship Program

(separate form to be filled for seat under Institute funding and project funding)

1. Name of faculty member proposing: **Prof. Kailash Singh**
2. Department/Centre **Chemical Engineering**
3. Topic on which work is proposed:

Reinforcement learning based machine learning control of a catalytic reactor

4. Preferred period of internship (after May 20th): **Between 22nd May 2024 to 16th July 2024**

5. Qualification of student (branch/semester of study): **B.Tech. (Chemical Engineering) 3rd year**

6. Brief description of work (300-500 words):

Catalytic reactors are used for producing many products across the industries. Optimizing their performance is crucial for maximizing yield, product purity, and energy efficiency. Conventional control methods rely on pre-defined mechanistic models, which may be challenging for complex reaction kinetics or unforeseen disturbances. Machine learning (ML) offers a promising alternative but requires significant data for training and testing.

The proposed work will use an approach using reinforcement learning (RL) for ML control of catalytic reactors. RL excels in situations with complex dynamics and limited pre-existing knowledge, making it ideal for this application.

This work has the potential to improve the control performance of catalytic reactors, leading to significant improvements in the chemical industry. The proposed approach can overcome the limitations of traditional methods and achieve optimal performance even under complex and unforeseen circumstances. The successful implementation of this work could pave the way for a new generation of intelligent and adaptive chemical processes.

The work will involve the following key points:

- Development of a dynamic mathematical model for the catalytic reactor. The model should capture the key reaction kinetics and process variables, such as temperature, pressure, feed composition, and product yields.
- Design a reinforcement learning agent using a deep neural network architecture to learn optimal control policies.
- The agent will receive sensor data from the simulated reactor as state information and take actions in the form of control adjustments.
- The reward function will be designed to incentivize the agent to maximize desired outcomes like product yield and purity while minimizing energy consumption and unwanted byproducts.
- Train the RL agent in the simulated environment by allowing it to explore the state space and learn from the consequences of its actions.
- Utilize appropriate RL algorithms like Deep Q-Networks (DQN) or Proximal Policy Optimization (PPO) for efficient training.
- Validate the trained agent's performance by comparing its control strategies with traditional methods like PID control across various operating conditions and unforeseen disturbances.

- Design a framework for integrating the RL agent with real-world catalytic reactors.
- This framework will involve translating sensor data from the reactor into suitable state information for the agent and translating the agent's control decisions into actionable adjustments in real-time.
- Compare the performance and robustness of RL control with traditional methods under realistic operating conditions.

7. Expected learning of student (upto 100 words):
   The students will learn the following:

   • Matlab, Python, and various libraries related to machine learning

   • A Reinforcement learning -based control strategy for catalytic reactors that can learn and adapt to changing conditions.

   • Development of mechanistic model of reactor performance

   • A framework for implementing RL control in real-world chemical processes.

   • Understanding the capabilities and limitations of RL for complex chemical reaction control.

8. Nature of work: (Experimental/simulation/mathematical modelling/data collection-analysis etc.): upto 50 words

   The work involves mathematical modelling, simulation, data analysis, etc.

9. If the seat is under project sponsored category: **No**
   a) If yes, number of seats announced:
   b) Name and ID no. of project from which stipend is chargeable

Signature of faculty member

Prof. Kailash Singh

Chemical Engineering

Note:

a) Proposing faculty member needs to be available at the Institute during the period internship is offered
b) No extra space or funding than the stipend will be provided by the institute for this purpose