

I-STEM Software Request - Guide Approval Form

User Details

- Name of Researcher: PRASHANT BHADULA
- User Type: ☒ Ph.D. Scholar ☐ Postdoctoral Researcher ☐ Bachelor's ☐ Masters
- Institution Name : MNIT JAIPUR
- Institutional Contact No: 9549650376
- Research Topic: Design of Permeable Reactive Barrier

Software Request Details

- Software Name: COMSOL
- Justification for Software Request: [Provide detailed explanation of how the software supports your research objectives]

Guide/Supervisor Approval

I, Sanyam Dangayach (Guide/Supervisor Name),

- Confirm that the above-mentioned researcher is affiliated with our institution
- Have reviewed the software request and its relevance to the researcher's academic work
- Approve the software request for research purposes

Approval Confirmation

- I approve the software request
- The software aligns with the researcher's research objectives
- The request meets the institutional research guidelines

Guide/Supervisor Signature: [Signature]

Date: 29/07/2025

Official Stamp/Seal: [Space for Institutional Stamp]

Dr. Sanyam Dangayach
Assistant Professor
Dept. of Civil Engg.
MNIT, JAIPUR

Important Notes

1. This form must be signed and scanned
2. The scanned copy must be uploaded with the software request
3. Electronic signatures are acceptable if from an official institutional email

Justification for Using COMSOL Multiphysics in the Design of a Permeable Reactive Barrier (PRB)

The design and optimisation of a Permeable Reactive Barrier (PRB) require a detailed understanding of coupled physical, chemical, and hydraulic processes occurring in subsurface environments. To effectively simulate these complex interactions, COMSOL Multiphysics offers a powerful and flexible platform that integrates multiple physics-based models.

1. Multiphysics Coupling Capability:

COMSOL allows for simultaneous modelling of fluid flow (Darcy's Law), solute transport (advection-dispersion), and reactive transport processes (e.g., sorption, precipitation-dissolution, redox reactions). This is crucial for accurately predicting the performance of PRBs, where multiple mechanisms interact in the removal of contaminants.

2. 2D/3D Geometry and Porous Media Simulation:

The subsurface environment and PRB geometry can be realistically modelled in both 2D and 3D. COMSOL enables the incorporation of heterogeneous soil layers, variable permeability, and site-specific dimensions, leading to more accurate field-scale simulations.

3. Reactive Transport Modelling:

Using the Transport of Diluted Species and Chemical Reaction Engineering interfaces, COMSOL can simulate the interaction of contaminants with reactive media (e.g., zero-valent iron, activated carbon, etc.). This includes first-order decay kinetics or more complex reactions such as ion exchange or surface complexation.

4. Time-Dependent and Steady-State Analysis:

The software supports both steady-state and transient analysis, enabling simulation of short-term behavior as well as long-term performance and breakthrough curves of contaminants across the PRB.

5. Parametric and Sensitivity Analysis:

COMSOL allows for systematic variation of design parameters such as barrier thickness, permeability, porosity, and reaction rates. This helps in optimising PRB design for maximum contaminant removal efficiency while minimising construction and maintenance costs.

6. Validation with Experimental or Field Data:

Model results can be validated with laboratory column study data or field monitoring results by calibrating the model through curve fitting and parameter tuning. COMSOL's visualisation tools help in comparing modelled concentration profiles with observed data.

7. Customisation and Scalability:

COMSOL's equation-based modelling interface enables customisation beyond built-in modules, allowing for user-defined kinetics or site-specific modifications. This makes it scalable for a wide range of contaminants and site conditions.