Outline for Mtech Stage II Project Report

1 The report will be written based on this outline

1. Chemical Process simulator:
   1.1. What is it.
   1.2. The three major components of a process simulator
      1.2.1. Compound Database.
      1.2.2. Thermodynamics
      1.2.3. Unit Operation Modules.
   1.3. Application of process simulators in education and industry.
2. Requirement: Need of an open source process simulator
   2.1. Commercial process simulator are very expensive, if used for educational purposes. Due to which most of the chemical engineering institutes exclude process simulation course from their curriculum
   2.2. Commercial process simulators are unaffordable for small and medium scale industries. Therefore most of them are poorly designed, which reduces the efficiency of the plant.
3. DWSIM: An open source steady state process simulator
   3.1. Follows sequential modular approach
   3.2. Intensive compound database.
   3.3. Good build in library of Unit operation and excellent thermodynamics.
   3.4. Contains extra utilities like graph plotting and optimization.
   3.5. Provides standalone thermodynamic library which can be used externally.
   3.6. Drawbacks:
      3.6.1. Not suitable for design problems.
      3.6.2. Most of the small scale industries consists of batch processes which needs dynamic simulation for which DWSIM cannot be used.
4. Openmodelica: An open source simulation environment for solving engineering models.
   4.1. Follows equation oriented approach.

4.2. Contains good built in solvers.
4.3. Excellent debugging features
4.4. Based on object oriented approach which has lots of advantages like code reuse and encapsulation.
4.5. Connectors: an advanced concepts for connecting object.
4.6. Provides Excellent GUI where each object can be directly connected with other through connectors. Therefore reduces manual coding.
4.7. Drawbacks: As it is a general software, there is no built in thermodynamics and unit operations.

5. Importing the Thermodynamic engine of DWSIM in Openmodelica.
   5.1. The two approaches used for the integration.
      5.1.1. Python-C Api approach.
      5.1.2. Client-Server approach (sockets).
   5.2. Comparison of the two approaches. Based on the time taken to simulate the same example.

6. Development of a built in Thermodynamic engine in Openmodelica itself.
   6.1. Requirement for a built in thermodynamic engine.
   6.2. Development of the three components of a thermodynamic engine.
      6.2.1. Development of Compound Database.
      6.2.2. Development of Thermodynamic Functions.
      6.2.3. Development of Thermodynamic Packages.
   6.3. Comparison with the earlier approaches.

7. Solved examples in Openmodelica by using built in thermodynamics.
   7.1. Generating Bubble point and Dew point curves for ethanol water system by using NRTL and UNIQUAC thermodynamic models.
   7.2. Steady state flash model capable of doing design calculations as well
   7.3. Dynamic flash model.
   7.4. Bubble batch distillation of Methanol and water from Ingham.
   7.5. Batch distillation with temperature controller for reflux.(part of PHD thesis by Efstathios S Iliopoulos)

8. Future Work
   8.1. Developing steady state and dynamic models of all the unit operation in Openmodelica.
   8.2. Validating the above models by comparing the simulated results with a commercial simulator.
   8.3. Documentation of the developed thermodynamics and unit modules.