Optimization of Ethanolamines Production with OpenModelica & CasADi

Murali Krishna Pilli & A S Anand
Imagine Simulation Technologies Pvt. Ltd.

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- Training Products and Services for Plant Operation and Safety
  - Tutorials and Generic Models for Process Concepts
  - Dynamic Real-time Simulation for Operations Training
- Production Analysis and Process Optimization
  - Data Based Model Building
- Plant Equipment (Asset) Performance Monitoring

Presenter

- Masters in Chemical Engineering
- Working as Technical Consultant
- Works on Product Research and Development

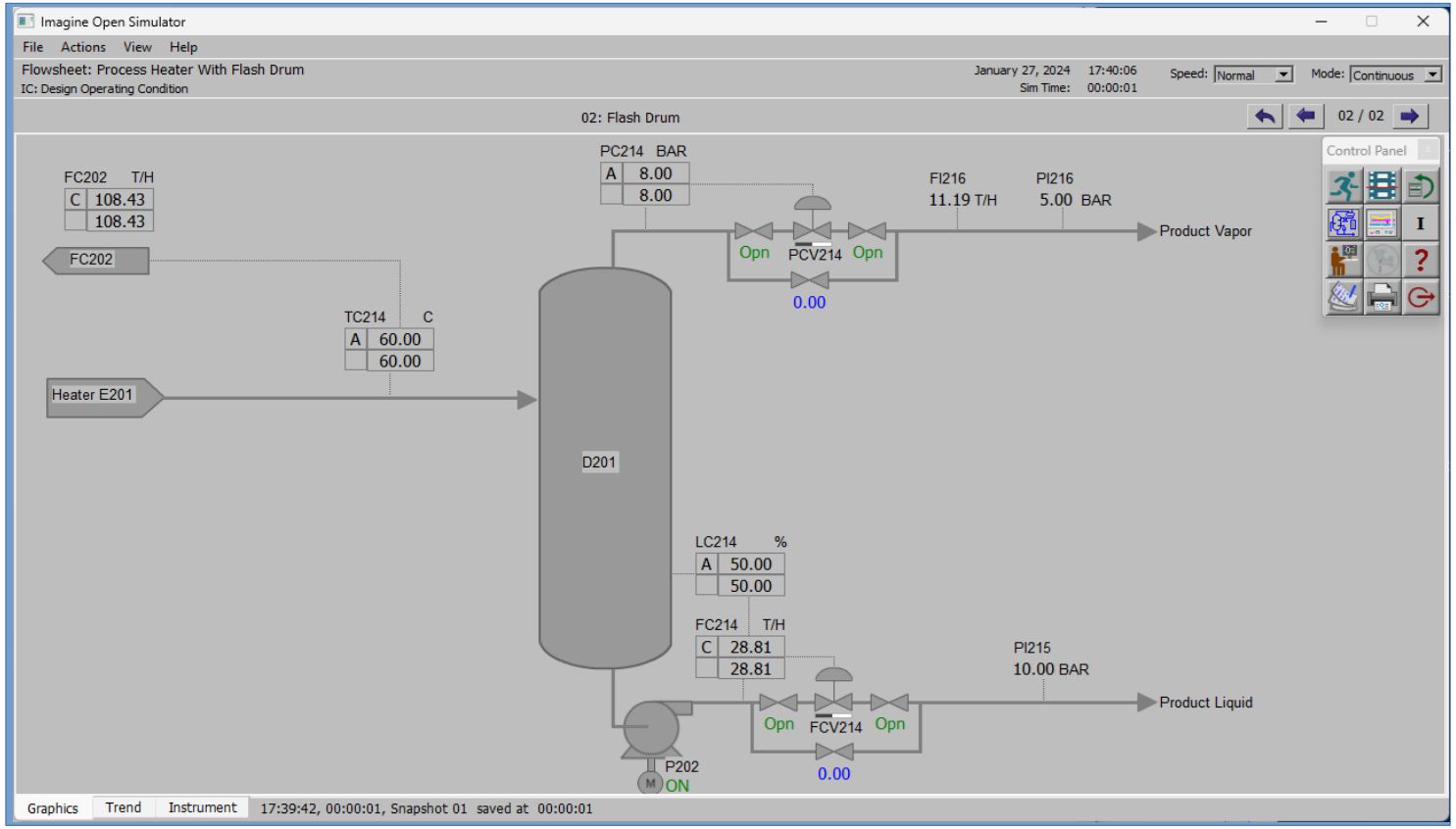
Imagine and OpenModelica

Imagine Simulation TECHNOLOGIES

Imagine's Modelica Based Simulator

- **Library with essential components**
- **Steady State and Dynamic Models**
- **Flowsheet exported as FMU**
- **OMSimulator with FMU Interfaces with Imagine's UI**

Imagine and OpenModelica



Our Optimization Objectives

➔ Use of open source tools that enable:

- **Optimization of chemical processes**
- **Optimal path for process transition**
- **Perform sensitivity analysis of key variables**
- **High level UI for ease of study**
- **Interface to Imagine's UI**

Target industry Oil&Gas, Chemicals, Petrochemicals, etc

Optimization & OpenModelica

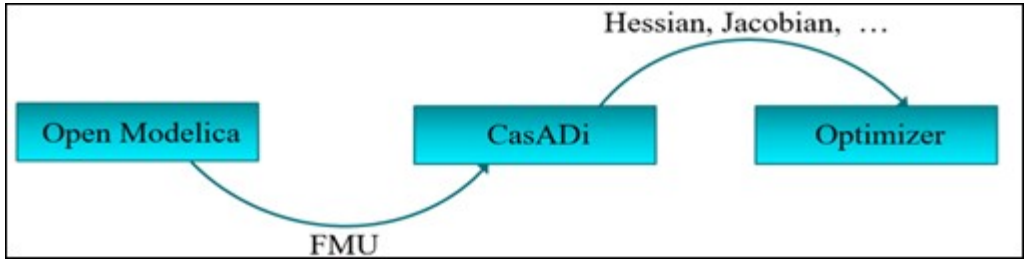
➔Optimization is supported in OpenModelica

- **Parameter Sweep**
- **Optimal Control**

➔Allows declaration of

- **Objective function**
- **Free variables and**
- **Constraints**

➔ Optimization problems cannot be exported to other platforms in the FMU format



- nonlinear optimization and algorithmic differentiation tool
- Modelica model is imported into CasADi using FMI format
- The Differential Algebraic Equations (DAE) from the FMU are read through the DaeBuilder class of CasADi
- CasADi facilitates creation of the goal function and constraints
- Explored the optimization of a real-world chemical process with the possibilities of building UI to present results

Ethanolamines (EAs)

- EthanolAmines (EAs) is a versatile group of Amino Alcohols
- EAs are predominantly used in Gas Treatment Processes
- The common EAs are
  - **MonoEthanolAmine (MEA)**
  - **DiEthanolAmine (DEA)**
  - **TriEthanolAmine (TEA)**

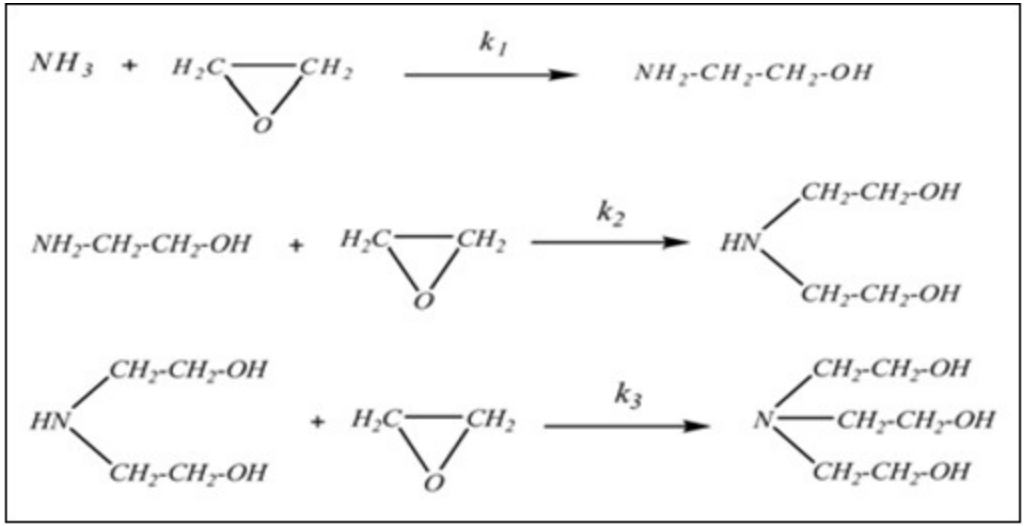
EAs Process: EO and NH3 Reactions

Three consecutive competing reactions, producing different EAs

$$EO + NH_3 \xrightarrow{K_1} MEA$$

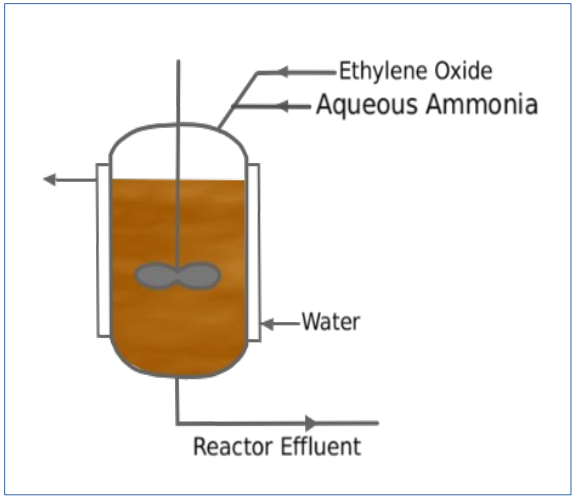
$$EO + MEA \xrightarrow{K_2} DEA$$

$$EO + DEA \xrightarrow{K_3} TEA$$

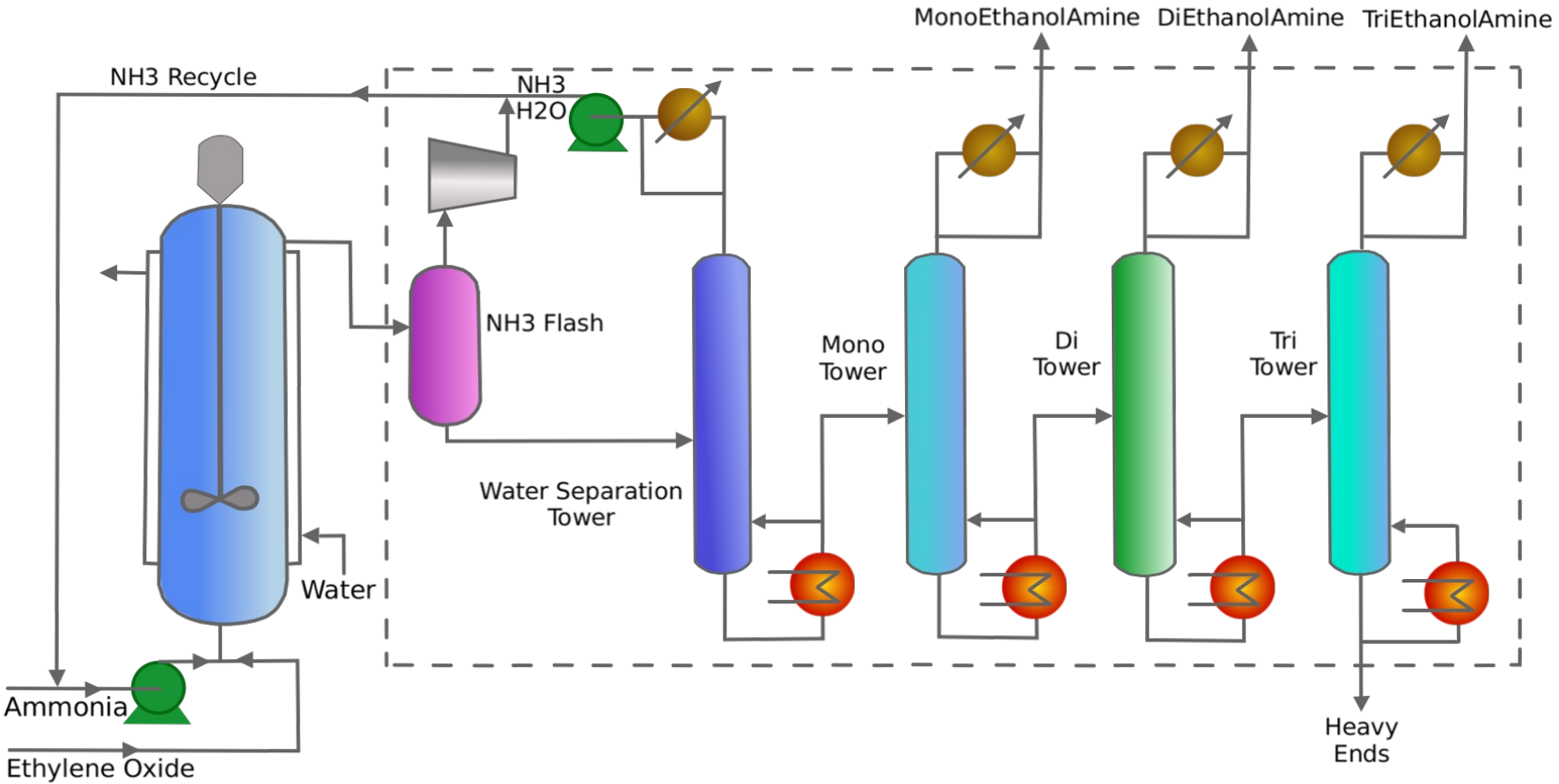


EAs Process: Features

- Synthesized by reacting Ethylene Oxide (EO) with Ammonia
- Liquid phase reaction
- Highly exothermic reaction
- Aqueous Ammonia processes use
  - **Ammonia concentrations from 45 to 55 wt%**
  - **Pressures up to 160 Bar**
  - **Temperatures up to 150°C**
  - **Excess Ammonia, up to 40 times EO**



EAs Process


MonoEthanolAmine
DiEthanolAmine
TriEthanolAmine
NH3 Recycle
NH3
H2O
NH3 Flash
Water Separation Tower
Mono Tower
Di Tower
Tri Tower
Water
Ammonia
Ethylene Oxide
Heavy Ends

Reactor Kinetics

$$EO + NH_3 \xrightarrow{K_1} MEA$$

$$EO + MEA \xrightarrow{K_2} DEA$$

$$EO + DEA \xrightarrow{K_3} TEA$$

$$K_1 = 7.845exp(-1150/RT)$$
$$K_2 = (8.151 - 0.051C_{H2Oout})K_1$$
$$K_3 = (14.81 - 0.196C_{H2Oout})K_1$$

$$r_{NH3} = \frac{dC_{NH3}}{dt} = -K_1 C_{NH3} C_{EO}$$

$$r_{EO} = \frac{dC_{EO}}{dt} = -K_1 C_{NH3} C_{EO} - K_2 C_{MEA} C_{EO} - K_3 C_{DEA} C_{EO}$$

$$r_{MEA} = \frac{dC_{MEA}}{dt} = K_1 C_{NH3} C_{EO} - K_2 C_{MEA} C_{EO}$$

$$r_{DEA} = \frac{dC_{DEA}}{dt} = K_2 C_{MEA} C_{EO} - K_3 C_{DEA} C_{EO}$$

$$r_{TEA} = \frac{dC_{TEA}}{dt} = K_3 C_{DEA} C_{EO}$$

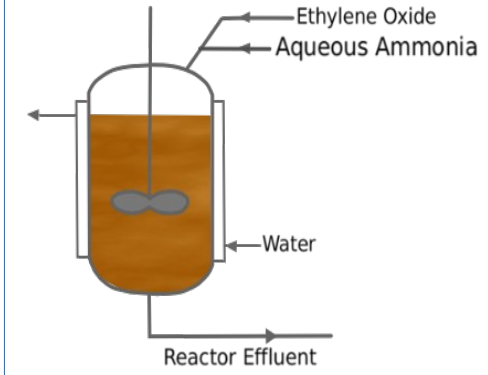
Continuous Stirred Tank Reactor (CSTR) Model

Equations

- Total mass balance
- Component balance including rate expressions

Variables

- Flow rate of inlets
- Outlet composition
- Water content in aqueous Ammonia
- Temperature
- Reactor volume



Optimization Requirement

- All three products are formed always, with different yields
- Dynamic market demand and value of products
- Process conditions to be varied to maximize the required product

Objective

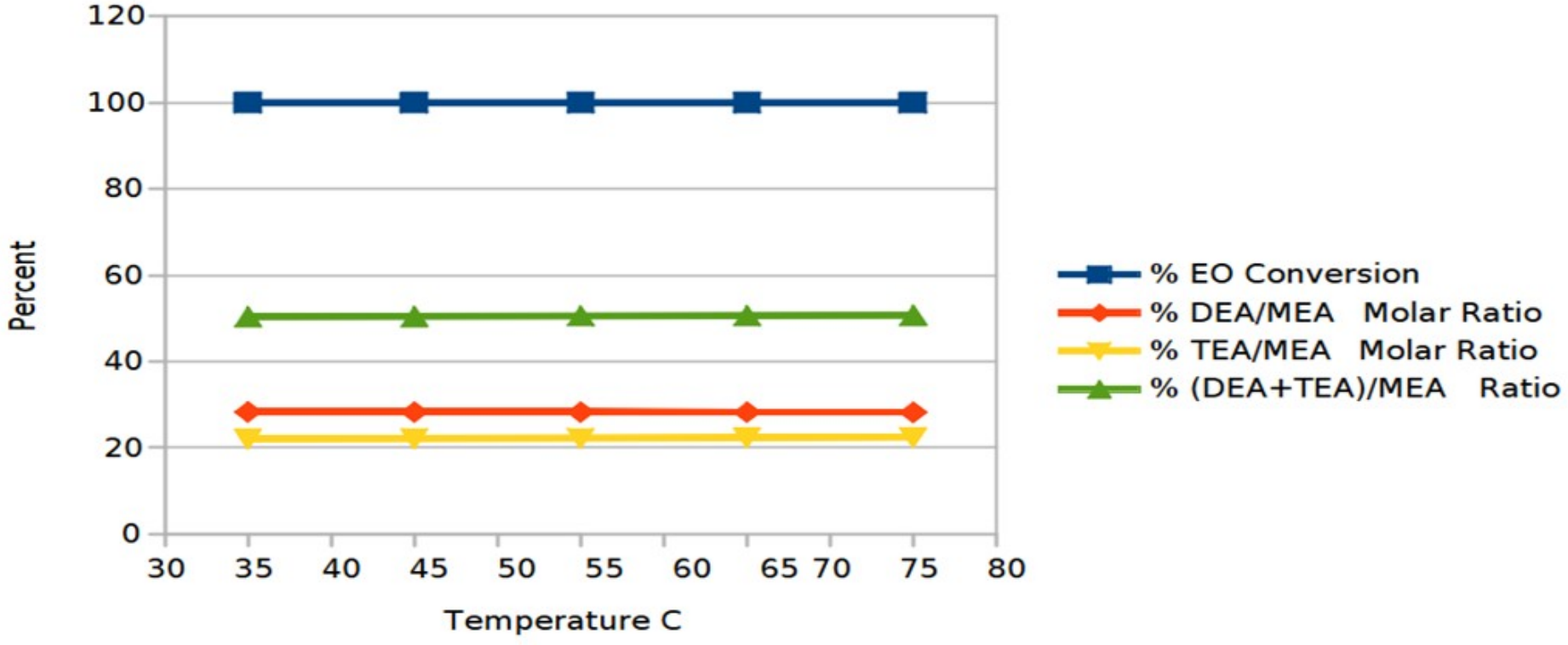
- **Maximize the MEA production at near complete conversion of EO**

Optimization Problem

- Optimization variables
  - **Reactor Temperature**
  - **Working volume of CSTR**
  - **Excess Ammonia**
- Minimize (DEA/MEA) and (TEA/MEA) at Reactor outlet, subject to
  - **Excess Ammonia of 10 to 30 mole ratio**
  - **Temperature of 35 to 75 C**
  - **Volume of 5 to 7 m3**

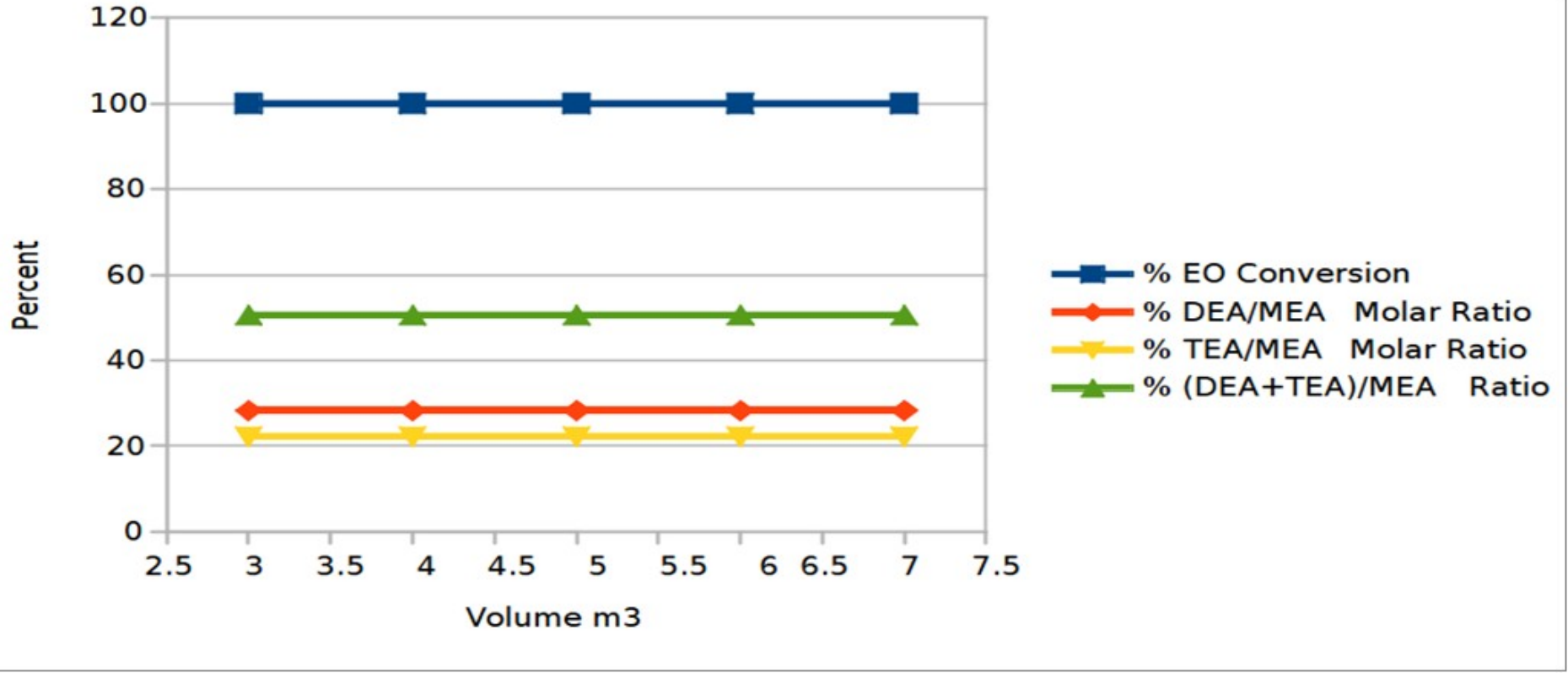
Sensitivity of Optimization Variables

Temperature sensitivity



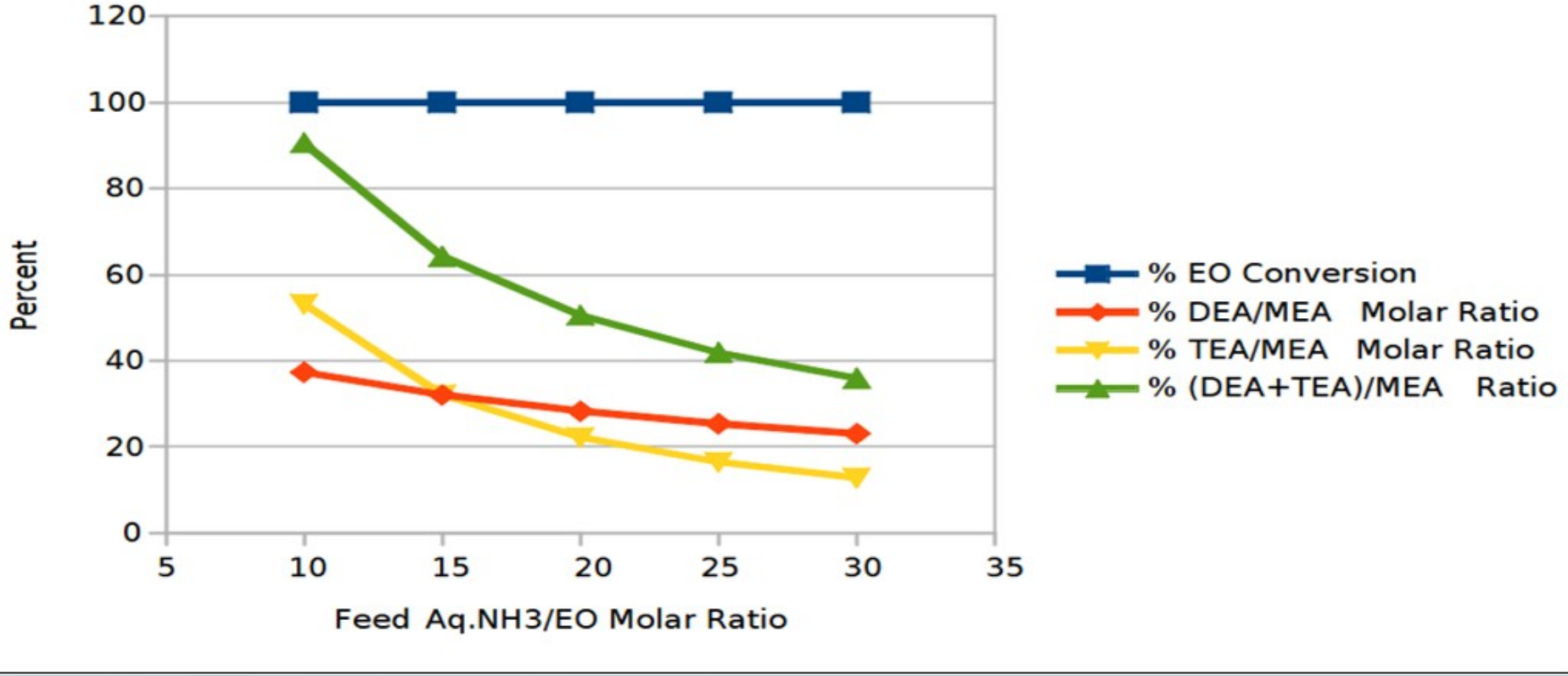
Sensitivity of Optimization Variables

Reactor Volume Sensitivity



Sensitivity of Optimization Variables

Excess NH3 Sensitivity



Optimum Reactor Conditions for Various Percent DEA/MEA Ratios

% DEA/MEA Molar Ratio	**23.2**	29.9	32.5	37.2
Temperature in C	**45.0**	47.0	46.5	44.0
Volume in m3	**3.6**	3.6	3.6	3.7
Feed Aq.NH3/EO Molar Ratio	**29.8**	17.8	14.5	10.0

Conclusions

- FMI support in CasADi utilized for the Optimization of Chemical Process
- Tool chain Modelica --> FMI --> CasADi is used to model and optimize
- Interfaced with Imagine's UI

Q & A

Contact Us

GET IN TOUCH

Address

Imagine Simulation Technologies Pvt. Ltd.
1B, 24, Third Cross Street
West C.I.T Nagar,
Nandanam, Chennai-600035 India

Call Us

+91 44 24333469

Mail Us

info@imaginesimtech.com