

Sandeep Prakash

Optimal Operation and Design of Thermal Energy Storage System

Specialization Project in Chemical Engineering

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Supervisor: Johannes Jäschke, Associate Professor IKP
Co-Supervisor: Mandar Thombre, PhD Candidate IKP

Department of Chemical Engineering
Faculty of Natural Science
Norwegian University of Science and Technology



Norwegian University of
Science and Technology

Cover page back

Dedicated to,

All the people who have been a part of my life, regardless of how long or for how brief.

*Thank You for the lessons you have taught me and the impact you have had,
whether you realize it or not.*

Table of contents

TABLE OF CONTENTS	IV
LIST OF FIGURES.....	VI
LIST OF TABLES.....	VII
CHAPTER 1.INTRODUCTION	1
<i>Central Themes</i>	<i>2</i>
CHAPTER 2.MODELLING TWO TANK THERMAL ENERGY STORAGE SYSTEM.....	4
2.1. TOPOLOGY	4
2.2. MODEL EQUATIONS	5
2.3. MODEL ANALYSIS	7
<i>Steady State</i>	<i>8</i>
<i>Open Loop Step Tests.....</i>	<i>10</i>
2.4. THE NEED FOR OPTIMIZATION	11
CHAPTER 3. OPEN LOOP OPTIMIZATION	13
3.1. TES OPTIMAL CONTROL PROBLEM.....	13
3.2. OPTIMAL CONTROL PROBLEM : ILLUSTRATIVE CASE.....	14
<i>The importance of Energy Quality for TES.....</i>	<i>16</i>
3.3. OPTIMAL CONTROL PROBLEM : REALISTIC CASE.....	17
3.4. DISCUSSION AND FURTHER IMPROVEMENTS	19
<i>Optimal Control Under Uncertainties</i>	<i>19</i>
<i>Linking TES to Electricity Markets</i>	<i>19</i>
CHAPTER 4. OPTMAL DESIGN PROBLEM	21
4.1. DESIGN MODEL.....	22
<i>Linking CAP_{tes} and Tank Volume (V_{tes_max})</i>	<i>22</i>
<i>Linking POW_{tes} and Area of Exchangers</i>	<i>23</i>
<i>Estimating Capital Cost (C_{CAPEX}) and Operating cost (C_{OPEX}).....</i>	<i>23</i>
4.2. OPTIMAL DESIGN WITHOUT UNCERTAINTY.....	24
<i>Illustrative Case</i>	<i>25</i>
CHAPTER 5. OPTIMAL DESIGN UNDER UNCERTAINTIES	27
5.1. TWO STAGE LINEAR STOCHASTIC PROGRAM WITH RECOURSE	27
5.2. TES DESIGN PROBLEM UNDER UNCERTAINTY	28
<i>Optimal Design : Illustrative Case.....</i>	<i>28</i>
<i>Optimal Design : Industrial Case</i>	<i>30</i>
5.3. DISCUSSION AND FURTHER IMPROVEMENTS	33

<i>Selection of Scenarios</i>	33
<i>Relaxing linear approximations in Objective Function</i>	33
<i>Relaxing the linear approximations in the Model</i>	34
REFERENCES	35
A1. TWO TANK TES MODEL	37
A1.A. CELL MODEL APPROXIMATION OF HEAT EXCHANGERS	37
A1.B. MASS AND ENERGY BALANCES	38
Energy Balance equations in Hex_Sup	38
Energy Balance equations in Hex_Con	38
Mass and Energy Balance across the storage tanks	39
A1.C. MODEL PARAMETERS	39
A2. DESIGN MODEL	40
A2.A. CAPITAL COST ESTIMATION	40
A3. SOURCE CODES – OPERATIONS MODEL	42
A3.A. PARAMETERS.M	42
A3.B. MODEL_DOT.M	42
A3.C. OPTIMAL_CONTROL_PROBLEM.M	43
A4. SOURCE CODES – DESIGN MODEL	50
A4.A. PARAMETERS.M	50
A4.B. TWO_STAGE_STOCHASTIC_PROGRAM.M	50

List of figures

Figure 1-1: The California Duck Chart [2]	1
Figure 2-1: Schematic of the Two Tank TES System	5
Figure 2-2 : Steady State Input Profile– q_c and q_h	8
Figure 2-3 : Steady State response – V_c and V_h	9
Figure 2-4 : Steady State response – Temperatures.....	9
Figure 2-5 : Input profile - Step change in q_c	10
Figure 2-6 : Step response – V_c and V_h	10
Figure 2-7 : Step response – Temperatures.....	11
Figure 3-1 : Illustrative case - Supply/ Demand profile	14
Figure 3-2 : Illustrative case – OCP Solution - input profile.....	15
Figure 3-3 : Illustrative case – TES tank volume profile.....	15
Figure 3-4 : Illustrative case - External utilities usage profile.....	16
Figure 3-5 : Realistic case – Supply/ Demand profile	17
Figure 3-6 : Realistic case – OCP Solution - input profile	18
Figure 3-7 : Realistic case – TES tank volume profile	18
Figure 3-8 : Realistic case - External utilities usage profile	19
Figure 4-1: Design Model.....	22
Figure 4-2 : Illustrative Design - Daily Profile (QSupply, QDemand).....	25
Figure 4-3 : Illustrative Design - TES Daily Operation.....	26
Figure 5-1 : Illustrative Stochastic Design - Daily Profile (QSupply, QDemand)	29
Figure 5-2 : Illustrative Stochastic Design - TES Daily Operation	30
Figure 5-3 : Industry Year Data.....	31
Figure 5-4 : Representative Weekly data – Supply and Demand Profiles.....	32
Figure 5-5 : Recourse Action for scenario 5.....	32
Figure 5-6 : Recourse Action for scenario 5	33
Figure A2-1 : Purchased cost relationship with Tank Volume.....	41
Figure A2-2 : Purchased cost relationship with Heat Exchanger Area	41

Appendix

Figure A 1-1: Cell model approximation for modelling Heat Exchanger	37
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List of tables

Table 2-1: Constant Temperatures assumed in the model.....	4
Table A2-1 : Tank Purchased Cost parameters.....	40
Table A2-2 : Exchanger Purchased Cost parameters.....	40

Chapter 1. Introduction

The share of energy being generated from renewable sources are on the rise, with forecasts estimating an expansion by another 50% between 2019 and 2024 as per the International Energy Agency [1]. Integration of an increasing proportion of renewables pose challenges to the grid operators due to their intermittent nature and uncertainty of production profiles. This issue is well illustrated using the California Independent System Operator (CAISO) Duck Chart shown in Figure 1-1, which shows the potential of photovoltaics to provide more energy than can be used by the system [2]. This termed as overgeneration risk, which occurs when conventional dispatchable resources cannot be backed down further to accommodate the supply of Variable Generation (VG).

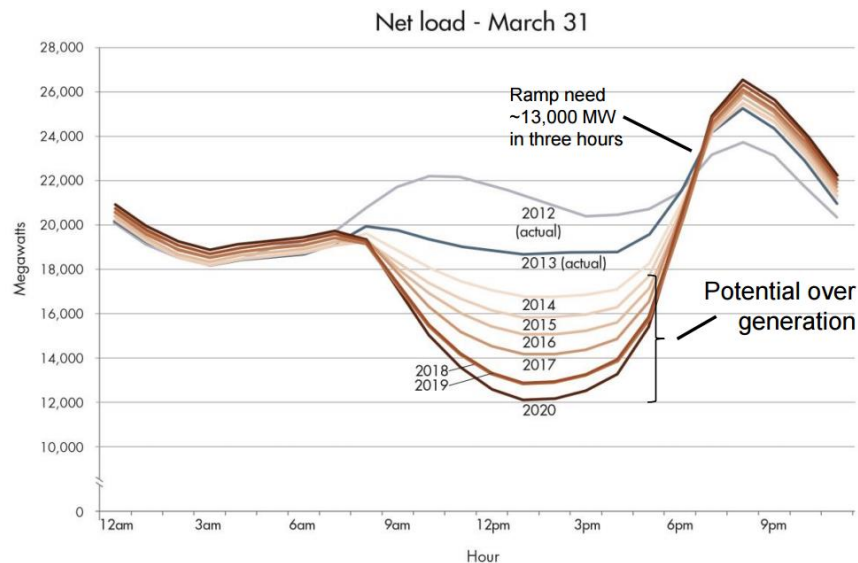


Figure 1-1: The California Duck Chart [2]

A relatively simple solution to the Over Generation risk is Curtailment, where the system operator would decrease the output from some of these VG' sources to below what it would normally produce. While curtailment is a relatively simple technical solution, it has the obvious undesirable effect of reducing the environmental and economical benefits offered by these renewable sources of energy. To enable greater integration of renewables into the energy mix, the electricity grid system needs additional flexibility, which can be achieved through various mechanisms like – Changes in operational practices, Institutional changes, Improved forecasting for renewable energy production and Storage among many others [3].

We focus our attention to energy storage as an enabler in the integration problem. There are many different kinds of energy storage, each with their pros and cons with no single technology emerging as a clear winner as to be universally applicable. A comprehensive review of the various technologies suitable for grid level energy storage can be found in [4].

Central Themes

Any energy storage system would operate in a dynamic fashion, charging up during periods of excess supply and discharging in periods of excess demand. Due to the dynamic nature of the process along with the uncertainties of future demand and supply profiles, problems related to the Optimal Capacity requirement for storage and of ensuring optimal operation are of immense interest.

Motivated by these, we try and explore these in the following two main parts in this report

- **Part 1** – deals with the **Operation Problem** which explores the question – *for a given dynamic process, what is the optimal control actions that can minimize some specified Operational objectives.*
- **Part 2** – deals with the **Design Problem** which explores the question – *given some information about uncertainties in the future, what is the Optimal Design decision we can take to minimize some specified Design objective.*

We explore these questions here in the context of a Thermal Energy Storage (TES) System, but wish to highlight that the concepts discussed or the approach followed is applicable to process systems in general and is agnostic in terms of applicability to different energy storage technologies.

Part 1

Operations Problem

Chapter 2. Modelling Two Tank Thermal Energy Storage System

We start by building a simple two tank TES system to explore the optimal operation of such an energy storage system when presented with a varying supply and demand profiles due to specific cooling and heating requirements of some process plants in a industrial cluster.

2.1. Topology

The two tank TES system stores energy as sensible heat of a TES fluid. In the topology presented in Figure 2-1, the supplier is a source of time varying thermal energy represented by the stream with flow q_{Sup} . The supplier provides the stream at a temperature T_{Sup_s} and requires the stream returned at temperature T_{Sup_r} . The supplier stream can be cooled by transferring heat to the TES through heat exchanger Hex_Sup and can be further cooled by a cooling water system by duty Q_{Dump} . Similarly, the Consumer side has a time varying thermal energy need represented by the stream with flow q_{Con} . This stream is provided at temperature T_{Con_s} and needs to be returned at temperature T_{Con_r} . The consumer stream is heated by the TES system through heat exchanger Hex_Con and can be further heated by an electric heater by duty Q_{Peak} .

To simplify our analysis, the supply and return temperatures of the supplier and consumer are assumed constant and the duty variations are represented by variations in flow q_{Sup} and q_{Con} . This simplifying assumption is realistic for the case of suppliers and consumers are industrial plants with Temperature specifications for their process streams, but can be relaxed in future work to better represent the integration of a TES system as a means of energy storage in other energy markets.

T_{Sup_s}	100	Deg C
T_{Sup_r}	40	Deg C
T_{Con_s}	10	Deg C
T_{Con_r}	70	Deg C

Table 2-1: Constant Temperatures assumed in the model

TES system is charged by heating the TES stream with flow q_c through Hex_Sup and storing the hot TES fluid in tank TES_Hot . All tanks are considered to be well mixed and the temperature in the hot tank is T_h . There is loss of heat to ambient from the hot tank at the rate of Q_{Loss_H} which is assumed propotional to the temperature in the tank. TES system discharges energy by releasing energy from stream q_h through Hex_Con and storing the cold TES fluid in tank TES_Cold .

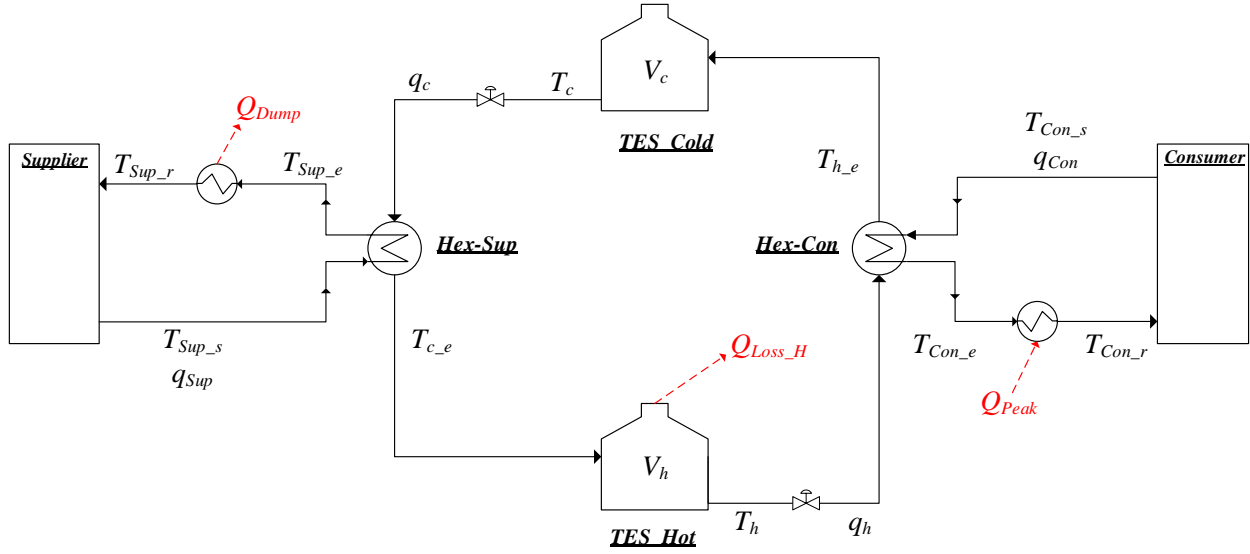


Figure 2-1: Schematic of the Two Tank TES System

In the model, Q_{Dump} is used when the supplier stream is not cooled to the return specification by the TES, which happens if there is not sufficient driving force across the heat exchanger. Similarly, Q_{Peak} is used when consumer stream is not heated to return specification by the TES. The usage of Q_{Peak} and Q_{Dump} has cost of C_{Dump} and C_{Peak} associated with them to represent costs associated with using external utilities in the case of an industrial cluster.

2.2. Model Equations

To model the TES system in Figure 2-1, we need to model the heat exchangers Hex_Sup and Hex_Con . The duty transferred for an ideal counter current heat exchanger is given as

$Q = UA\Delta T_{LMTD}$. The Log Mean Temperature Difference (LMTD) causes issues in iterative

equation solving schemes due to the indeterminate form of the logarithmic function and undefined derivatives at intermediate solver values [5]. Various approximations of LMTD are used in practice during design as described by Paterson [5], Underwood [6] or Chen [7].

A widely accepted approach to model the dynamic behaviour of heat exchangers is to use cell based dynamic models where a simple heat exchange cell is defined as two perfectly stirred tanks, exchanging heat only with each other through a dividing wall [8]. A review of the important model features for the dynamics of heat exchangers by Mathisen can be found in [9]. We approximate the heat exchangers as a series of thermally coupled Continuously Stirred Tanks (details of discretization and identifiers for new states in Appendix A1.a), with the heat

exchangers modelled as n cells in series ($nCell = 3$). We write the mass and energy balance for the Two Tank TES system in Appendix A1, where the relevant assumptions considered are also described during modelling. We get the set of Ordinary Differential Equations (2.8) to (2.8) below in consistent units.

Energy Balance across the Heat Exchangers Hex_Sup and Hex_Con , we get,

$$\begin{aligned}
\frac{dT_{Sup_e(1)}}{dt} &= \frac{q_{Sup}}{V_{Cell}} (T_{Sup_s} - T_{Sup_e(1)}) - \frac{h_{Cell} A_{Cell}}{\rho_{Sup} V_{Cell} C_{P_Sup}} (T_{Sup_e(1)} - T_{c_e(3)}) \\
\frac{dT_{Sup_e(2)}}{dt} &= \frac{q_{Sup}}{V_{Cell}} (T_{Sup_e(1)} - T_{Sup_e(2)}) - \frac{h_{Cell} A_{Cell}}{\rho_{Sup} V_{CSTR} C_{P_Sup}} (T_{Sup_e(2)} - T_{c_e(2)}) \\
\frac{dT_{Sup_e(3)}}{dt} &= \frac{q_{Sup}}{V_{Cell}} (T_{Sup_e(2)} - T_{Sup_e(3)}) - \frac{h_{Cell} A_{Cell}}{\rho_{Sup} V_{Cell} C_{P_Sup}} (T_{Sup_e(3)} - T_{c_e(1)})
\end{aligned} \tag{2.1}$$

$$\begin{aligned}
\frac{dT_{c_e(1)}}{dt} &= \frac{q_c}{V_{Cell}} (T_c - T_{c_e(1)}) + \frac{h_{Cell} A_{Cell}}{\rho_c V_{Cell} C_{P_c}} (T_{sup_e(3)} - T_{c_e(1)}) \\
\frac{dT_{c_e(2)}}{dt} &= \frac{q_c}{V_{Cell}} (T_{c_e(1)} - T_{c_e(2)}) + \frac{h_{Cell} A_{Cell}}{\rho_c V_{Cell} C_{P_c}} (T_{sup_e(2)} - T_{c_e(2)}) \\
\frac{dT_{c_e(3)}}{dt} &= \frac{q_c}{V_{Cell}} (T_{c_e(2)} - T_{c_e(3)}) + \frac{h_{Cell} A_{Cell}}{\rho_c V_{Cell} C_{P_c}} (T_{sup_e(1)} - T_{c_e(3)})
\end{aligned} \tag{2.2}$$

$$\begin{aligned}
\frac{dT_{h_e(1)}}{dt} &= \frac{q_h}{V_{Cell}} (T_h - T_{h_e(1)}) - \frac{h_{Cell} A_{Cell}}{\rho_h V_{Cell} C_{P_h}} (T_{h_e(1)} - T_{Con_e(3)}) \\
\frac{dT_{h_e(2)}}{dt} &= \frac{q_h}{V_{Cell}} (T_{h_e(1)} - T_{h_e(2)}) - \frac{h_{Cell} A_{Cell}}{\rho_h V_{Cell} C_{P_h}} (T_{h_e(2)} - T_{Con_e(2)}) \\
\frac{dT_{h_e(3)}}{dt} &= \frac{q_h}{V_{Cell}} (T_{h_e(2)} - T_{h_e(3)}) - \frac{h_{Cell} A_{Cell}}{\rho_h V_{Cell} C_{P_h}} (T_{h_e(3)} - T_{Con_e(1)})
\end{aligned} \tag{2.3}$$

$$\begin{aligned}
\frac{dT_{Con_e(1)}}{dt} &= \frac{q_{Con}}{V_{Cell}} (T_{Con_s} - T_{Con_e(1)}) + \frac{h_{Cell} A_{Cell}}{\rho_{Con} V_{Cell} C_{P_Con}} (T_{h_e(3)} - T_{Con_e(1)}) \\
\frac{dT_{Con_e(2)}}{dt} &= \frac{q_{Con}}{V_{Cell}} (T_{Con_e(1)} - T_{Con_e(2)}) + \frac{h_{Cell} A_{Cell}}{\rho_{Con} V_{Cell} C_{P_Con}} (T_{h_e(2)} - T_{Con_e(2)}) \\
\frac{dT_{Con_e(3)}}{dt} &= \frac{q_{Con}}{V_{Cell}} (T_{Con_e(2)} - T_{Con_e(3)}) + \frac{h_{Cell} A_{Cell}}{\rho_{Con} V_{Cell} C_{P_Con}} (T_{h_e(1)} - T_{Con_e(3)})
\end{aligned} \tag{2.4}$$

The mass and energy balance in the tanks, we get,

$$\frac{dT_c}{dt} = \frac{q_h}{V_c} (T_{h-e} - T_c) \quad (2.5)$$

$$\frac{dT_h}{dt} = \frac{q_c}{V_h} (T_{c-e} - T_h) - \frac{U_{hot_tank} A_{hot_tank} (T_h - T_{amb})}{V_h \rho_{TES} C_{p_TES}} \quad (2.6)$$

$$\frac{dV_c}{dt} = q_h - q_c \quad (2.7)$$

$$\frac{dV_h}{dt} = q_c - q_h \quad (2.8)$$

Similarly, for the Supplier and Consumer Temperature constraints that need to be satisfied, we get the constraints,

$$q_{Sup} \rho_{Sup} C_{p_Sup} T_{Sup-r} = q_{Sup} \rho_{Sup} C_{p_Sup} T_{Sup-e} - Q_{Dump} \quad (2.9)$$

$$q_{Con} \rho_{Con} C_{p_Con} T_{Con-e} + Q_{Dump} = q_{Con} \rho_{Con} C_{p_Con} T_{Con-r} \quad (2.10)$$

In the model, we have the 16 state variables

$$x = \left[T_{Sup-e(1/2/3)} \quad T_c \quad T_h \quad T_{c-e(1/2/3)} \quad T_{h-e(1/2/3)} \quad T_{Con-e(1/2/3)} \quad V_c \quad V_h \right]^T \quad (2.11)$$

the 4 input variables

$$u = \left[Q_{Dump} \quad Q_{Peak} \quad q_c \quad q_h \right]^T \quad (2.12)$$

And the 2 time varying parameters, which are givens to the system

$$p = \left[q_{Sup} \quad q_{Con} \right]^T \quad (2.13)$$

Other fixed parameters used in the model are given in Appendix A1.c.

2.3. Model Analysis

We check the model developed in the section above for any errors, by simulating it with some simple input profiles. The TES is assumed to be at steady state for the first value of Supply and demand flows at the beginning of the simulation. The total inventory is chosen such that it could

be accommodated in a single tank. Since the levels in the tank do not have any steady state effect, the initial inventory in the hot tank is taken as 150 m³ with the remaining inventory in the cold tank so that TES always starts at the same initial charge to enable a fair comparison between different cases. In this chapter, we assume there is no heat loss from the hot tank to first build an intuitive understanding of the system before introducing further complexities.

Steady State

A TES system operates in a cyclic mode, but here we simulate the model with steady state values to check for any errors during model development. We provide steady state inputs

$$u_0 = [503.87 \quad 503.87 \quad 60 \quad 60]^T \quad (2.14)$$

corresponding to variables in the order presented in equation (2.12) and observe the model response for 48 hours with a dt of 1 hour. Inputs q_c and q_h are held constant at 60 m³/hr as shown in Figure 2-2.

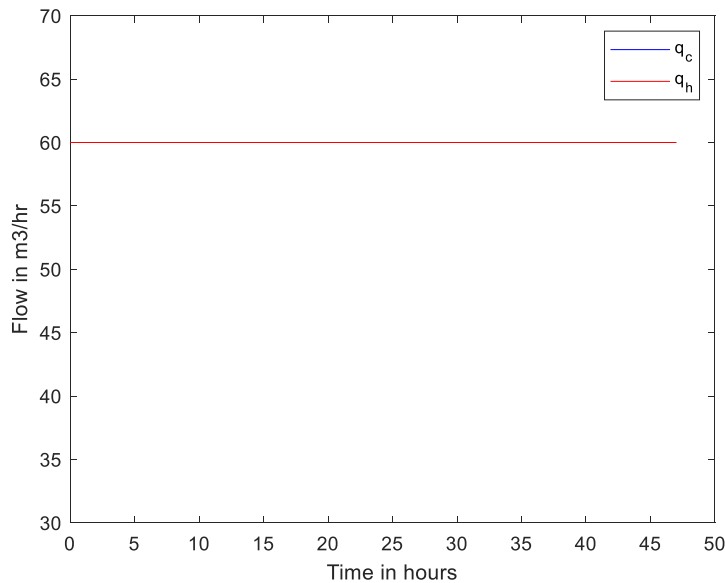


Figure 2-2 : Steady State Input Profile– q_c and q_h

We observe the response of V_c and V_h in Figure 2-3, which do not vary from the initial state.

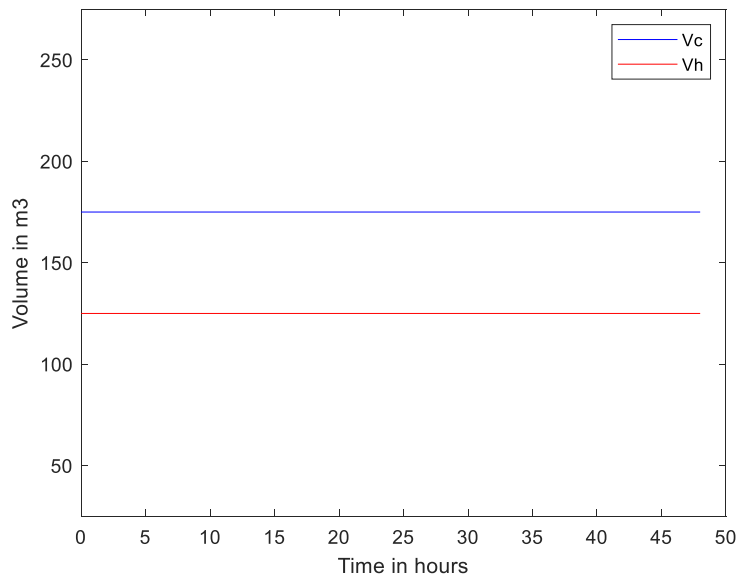


Figure 2-3 : Steady State response – V_c and V_h

Response in temperatures are also in Figure 2-4, which also as can be seen to not deviate from the initial state.

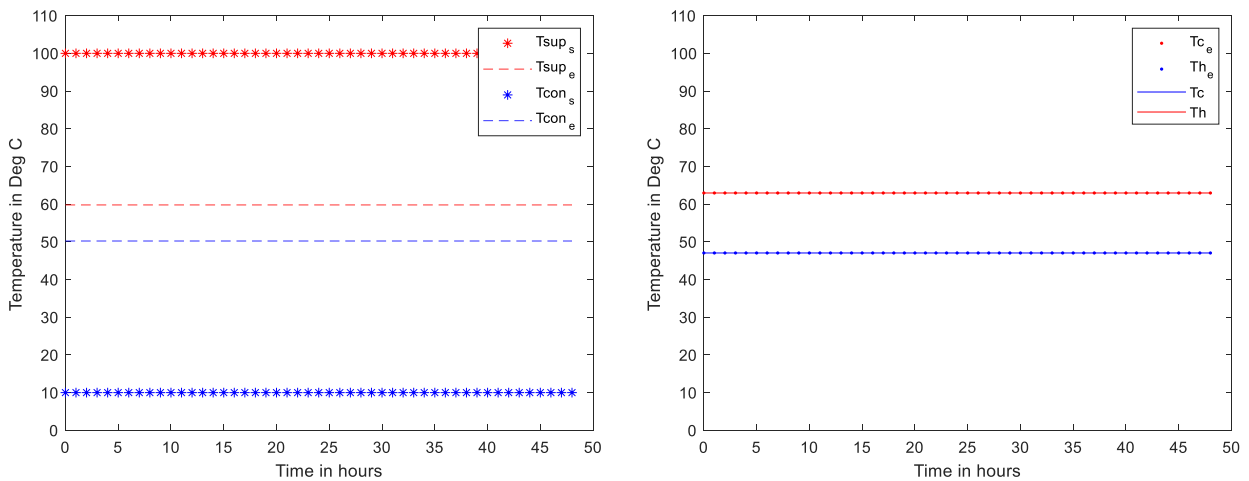


Figure 2-4 : Steady State response – Temperatures

For ease of understanding, we have followed the convention of plotting the relatively hot stream properties in red while the relatively cold stream properties are plotted in blue. For example – While plotting tank volumes, the relatively hot stream property V_h is in red and the relatively cold stream property V_c is in blue. Similarly, while plotting temperatures around heat

exchangers, the relatively hot stream properties - T_{Sup_s} , T_{Sup_r} , T_h and T_{c_e} are in red while the relatively cold stream properties - T_{Con_s} , T_{Con_e} , T_c and T_{h_e} are in blue.

Open Loop Step Tests

We make a step change in q_c as in Figure 2-5 to observe the response in all the states.

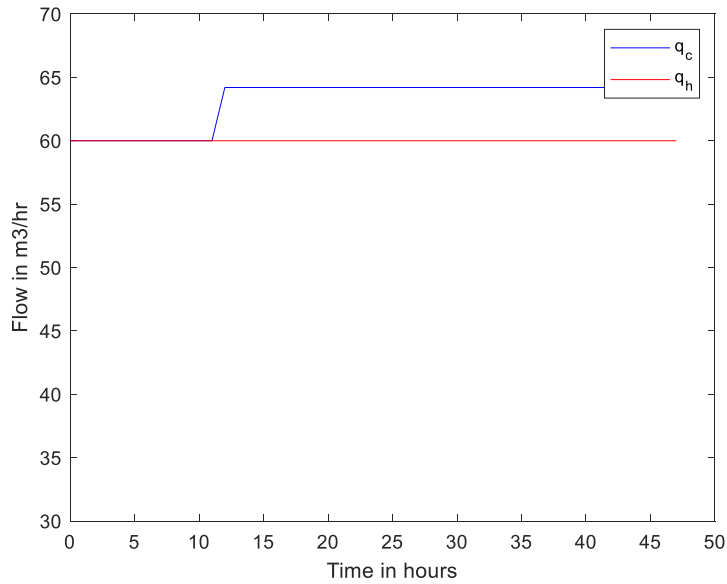


Figure 2-5 : Input profile - Step change in q_c

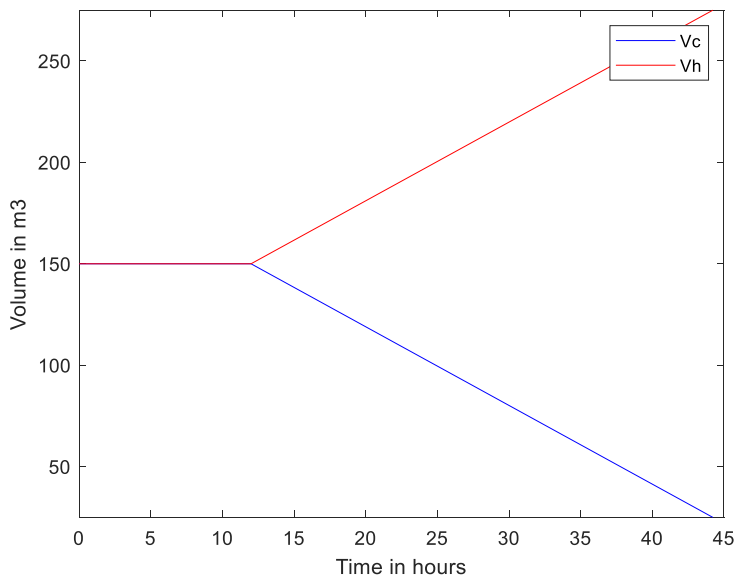


Figure 2-6 : Step response - V_c and V_h

As expected, we see the integrating response in tank volumes in Figure 2-6. Since we have increased the cold side flow of Hex_Sup , we see a first order response in hot side temperature T_{Sup_e} . Since there is more cold flow, T_{c_e} reduces, which leads to drop in hot tank temperature T_h . Although the flow of hot side in Hex_Con has not changed, due to the drop in temperature T_h of the hot side, we see a drop in the cold side exit temperature T_{Con_e} and also hot side exit temperature T_{h_e} . The temperature response to the step change in q_c is shown in Figure 2-7.

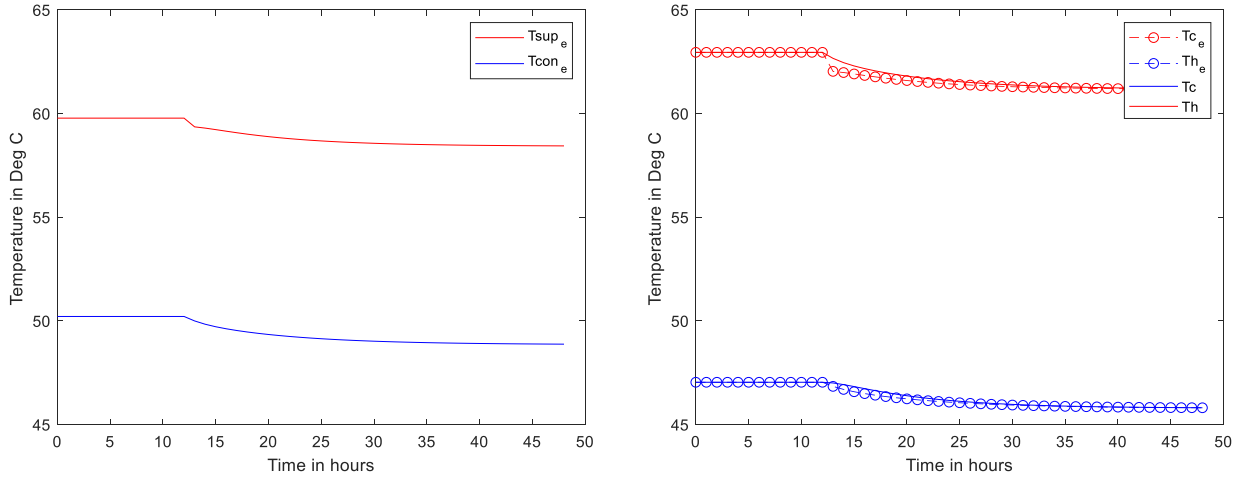


Figure 2-7 : Step response – Temperatures

2.4. The need for Optimization

The operation of the TES system is cyclic in nature - Charging during periods of excess thermal energy supply and Discharging during periods of insufficient supply. We consider a simple diurnal system which charges during the day and discharges during night. A comprehensive review of various types of TES systems and their operations can be found in [10].

Our objective is to satisfy the supplier and consumer temperature requirements with minimum reliance on Q_{Dump} and Q_{Peak} while being within flow and volume constraints in the TES. The primary operations decisions at any time t are the flows $q_c(t)$ and $q_h(t)$, with $Q_{Dump}(t)$ and $Q_{Peak}(t)$ used to achieve further cooling/ heating of the supplier/ consumer streams not achieved by the TES. These decisions are not very intuitive due to the complex coupled nature of how the primary decision variables have an impact on all the states as demonstrated in Section 2.3.

As an example, suppose we choose a low q_c , we will have a high exit temperature T_{c_e} (Approaches T_{Sup_s} when q_c tends to zero), but we will end up using larger Q_{Peak} since we are not transferring much heat to the TES. On the other extreme, if we try to drive Q_{Peak} to zero, we risk

having large q_c which would risk filling the hot tank at low temperature. A similar argument can be made for the decision of q_h on the consumer side.

Furthermore, since we consider heat loss from the hot tank, completely filling the hot tank early in the day has the adverse effect of larger heat loss for longer and ending up with a low temperature T_h during the night as compared to if we had decided to charge the TES towards the later part of the day.

Since we wish to deal with a wide variety of Supplier and Consumer profiles, we will have different and switching active constraints. Hence we formulate an optimization problem to ensure optimality in operation under all possible cases. Furthermore, the optimization problem lets us expand us to include variations in the cost of Q_{Dump} and Q_{Peak} and more importantly to deal with uncertainties in the future Supplier and Consumer Profiles through robust and stochastic formulations [11] of the optimization problem.

Chapter 3. Open Loop Optimization

In the previous chapter, we built a dynamic model for the two tank TES system and put forward the need for a dynamic Optimal Control Problem (OCP). The general form of an OCP is,

$$\min_{\mathbf{x}(t), \mathbf{u}(t)} \int_{t_0}^{t_f} \ell(\mathbf{x}(t), \mathbf{u}(t)) dt \quad (3.1.a)$$

$$s.t \quad \dot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p}(t)) \quad (3.1.b)$$

$$\mathbf{g}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p}(t)) \leq 0 \quad (3.1.c)$$

$$\mathbf{x}(t_0) = \mathbf{x}_t \quad (3.1.d)$$

$$\mathbf{x} \in \mathcal{X}, \mathbf{u} \in \mathcal{U} \quad (3.1.e)$$

where $\mathbf{x}(t) \in \mathbb{R}^{n_x}$ are the states, $\mathbf{u}(t) \in \mathbb{R}^{n_u}$ is the control inputs and $\mathbf{p}(t) \in \mathbb{R}^{n_p}$ is the model parameters and disturbances. ODE of the process model is $\mathbf{F} : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p}$ to \mathbb{R}^{n_x} .

To solve this as a standard optimization problem, we discretize it as a finite dimensional Nonlinear Programming Problem (NLP) divided as N equally spaced sampling intervals. The discretization can be performed using various approaches like single shooting, Multiple shooting or Direct Collocation which is better described in Chapters 9 and 10 of Biegler [12]. Then we get the OCP as a standard NLP of the form,

$$\min_{\mathbf{x}_k, \mathbf{u}_k} \sum_{k=0}^{N-1} \ell(\mathbf{x}_k, \mathbf{u}_k) \quad (3.2.a)$$

$$s.t \quad \mathbf{x}_{k+1} = \mathbf{f}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{p}_k) \quad \forall k \in \mathcal{K} \quad (3.2.b)$$

$$\mathbf{g}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{p}_k) \leq 0 \quad \forall k \in \mathcal{K} \quad (3.2.c)$$

$$\mathbf{x}_0 = \mathbf{x}_t \quad (3.2.d)$$

$$\mathbf{x}_k \in \mathcal{X}, \mathbf{u}_k \in \mathcal{U} \quad \forall k \in \mathcal{K} \quad (3.2.e)$$

where the discretized process model is $\mathbf{f} : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p}$ to \mathbb{R}^{n_x} .

3.1. TES Optimal Control Problem

The objective function of the OCP for the two tank TES system can be defined as the total OPEX during the control horizon which needs to be minimized. Mathematically, this can be shown as

$$\min_{\mathbf{x}_k, \mathbf{u}_k} \sum_{k=0}^{N-1} c_{dump}(k) Q_{Dump}(k) + c_{peak}(k) Q_{Peak}(k) \quad (3.3)$$

Where $c_{dump}(k)$ and $c_{peak}(k)$ are the costs for using QDump and QPeak respectively, which could vary with time (We consider them constant here to keep the discussion simple).

We use multiple shooting approach to discretize the problem here since the model equations are fairly nonlinear in the state variables, and would be poorly conditioned to be effectively solved using a sequential strategy like Single shooting. We solve the OCP in MATLAB using the CasADi symbolic framework [13], which makes our code implementation simple and links well into available Nonlinear solvers like IPOPT [14]. The Matlab source code for the implementation of the OCP can be found in Appendix A3.c. We discuss the solution of the OCP with an illustrative case below.

3.2. Optimal Control Problem : Illustrative Case

Let us consider a simple profile for heat supply and demand (represented as flows of supplier and consumer flows under constant battery limit temperatures in our case) as shown in Figure 3-1 for 2 days. We can see that there is excess supply during the first 24 hours which equals the shortfall in supply during the last 24 hours. We expect the TES to charge during day 1 and discharge completely during day 2, but are unsure of the optimal profile of q_c and q_h to achieve this.

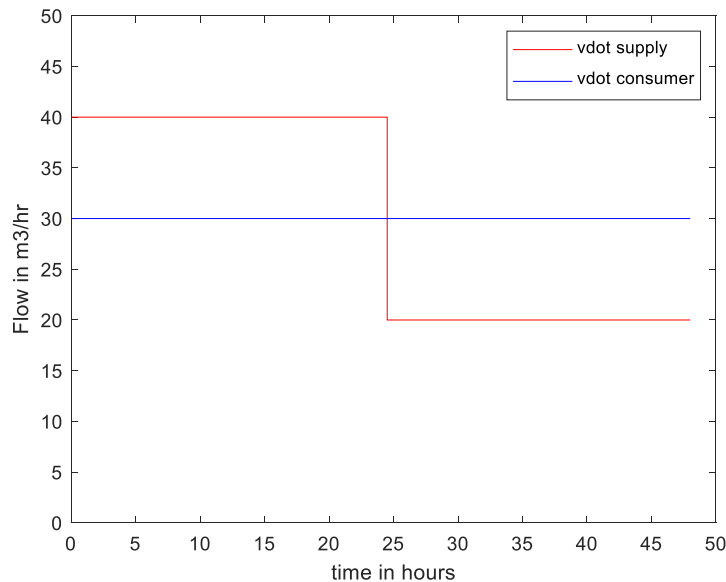


Figure 3-1 : Illustrative case - Supply/ Demand profile

Assuming the TES to be initially at the optimal steady state corresponding to the first value of Supply and demand flows with the inventory in the hot tank at 150 m³, we solve the OCP and get the profile for q_c and q_h as shown in Figure 3-2.

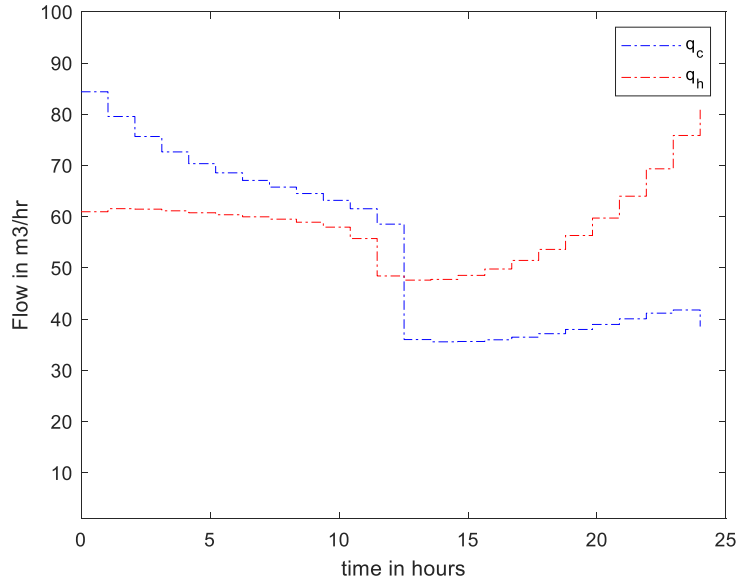


Figure 3-2 : Illustrative case – OCP Solution - input profile

We can see from Figure 3-3 that the TES is charging up during the first day (represented by the build up of volume in the hot tank) and discharging completely during the second day.

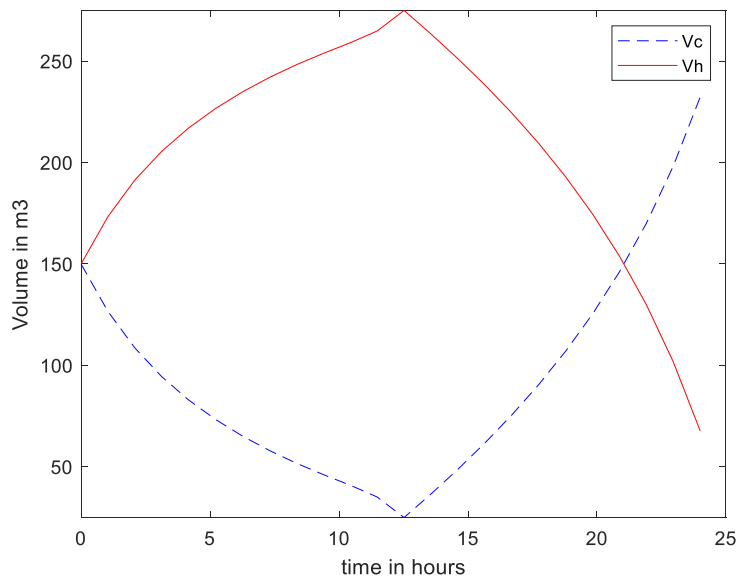


Figure 3-3 : Illustrative case – TES tank volume profile

Even though total supply and demand for thermal energy is equal, we can see that we still rely on both external cooling and heating utilities as seen in Figure 3-4. This is due to the parameters of the TES which are already decided during design (TES Tank Volume and Heat Exchanger Area in our case) and the nonlinear impact these have on the TES system to store and transfer energy.

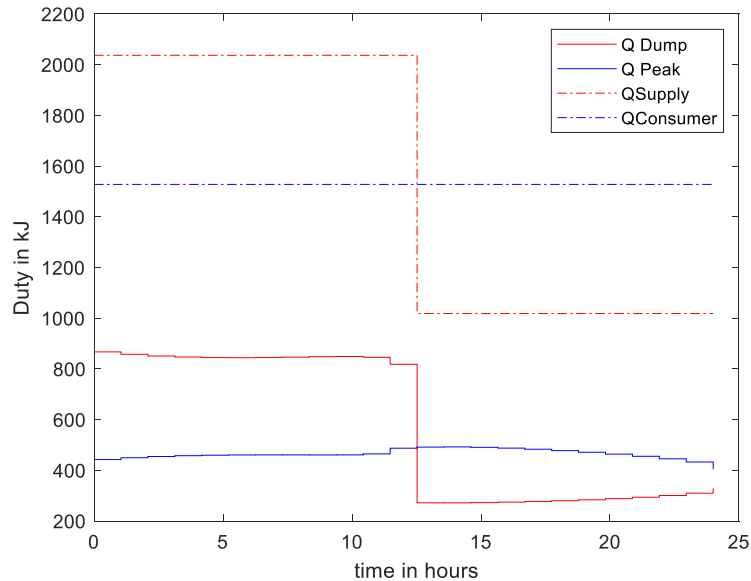


Figure 3-4 : Illustrative case - External utilities usage profile

The importance of Energy Quality for TES

With a fixed area for the heat exchangers, if we try to reduce Q_{Dump} by flowing higher q_c , we would need a higher capacity of for the hot tank to store this volume. Even if we had a large enough tank to accommodate this extra flow of q_c to drive Q_{Dump} to zero, the exit temperature of the TES Fluid from Hex_{Sup} (T_{c_e}) would be lower than earlier. This would result in a colder storage temperature T_h in the hot tank. A lower T_h reduces the ability of the TES to transfer energy to the consumer stream across Hex_{Con} , which would result in a larger dependence on Q_{Peak} to ensure the required return temperature for the consumer is met. This issue clearly demonstrates the importance of the quality of energy stored (Temperature of TES fluid in hot tank) along with the quantity of energy stored (total amount of Duty stored) in the TES. The quality of energy stored is improved with a larger heat exchanger area (with T_{c_e} reaching T_{Sup_s} when area approaches infinity) and the maximum quantity with the capacity of the tank.

It is impractical to assume an infinite area for the heat exchanger or capacity for the tanks, and we will discuss how these design parameters could be optimally chosen in Part 2 of the report – The Design Problem.

3.3. Optimal Control Problem : Realistic Case

We have seen how even for a simple Supply/ Demand profile as considered in the previous section, the choice of the optimal control profiles are not simple. We now demonstrate the solution of the OCP for a more realistic profile.

We started our discussion with the motivation of integrating renewable sources of energy into the electricity grid and the concept of the California Duck chart. So let us consider the profiles for renewables and the total load from the duck curve to represent Q_{Supply} and Q_{Demand} profiles in our thermal case. We scale the original data points and shift the Q_{Supply} profile up to match the total daily demand as shown in Figure 3-5. We could consider this case similar to the Concentrated Solar Thermal Plant integrated with TES system as presented by Kody Powell in [15].

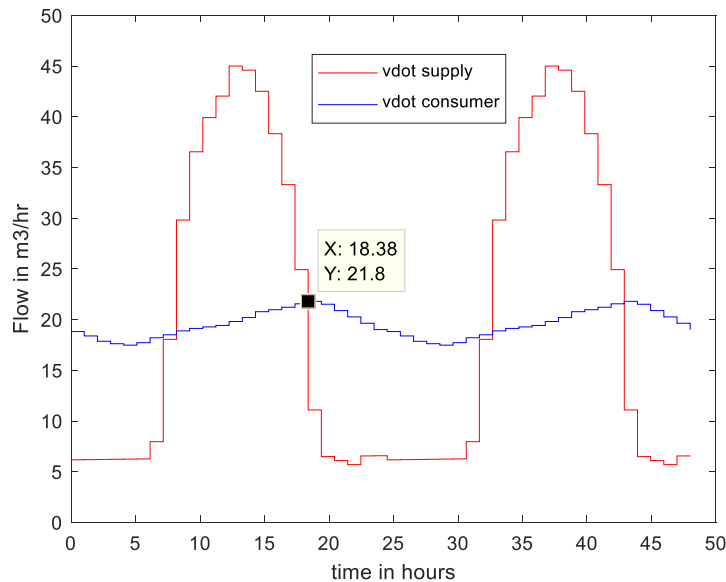


Figure 3-5 : Realistic case – Supply/ Demand profile

We observe a similar pattern of charging and discharging cycles in the solution of the OCP in Figure 3-6 and Figure 3-7.

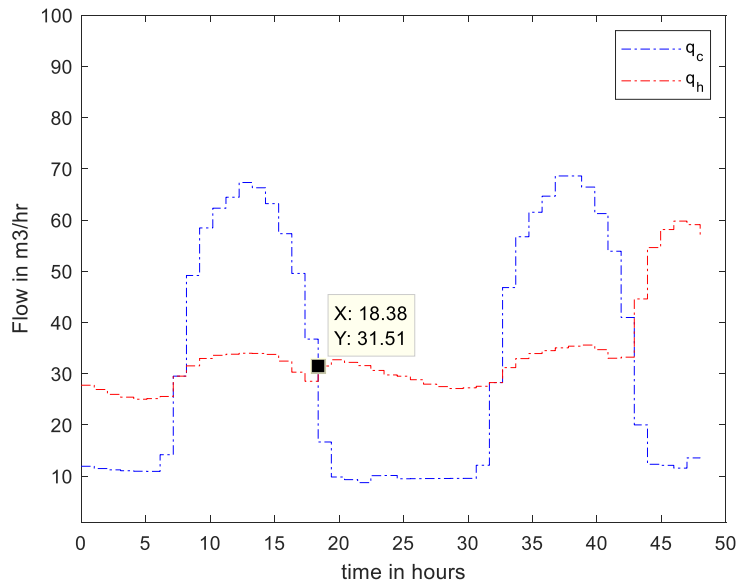


Figure 3-6 : Realistic case – OCP Solution - input profile

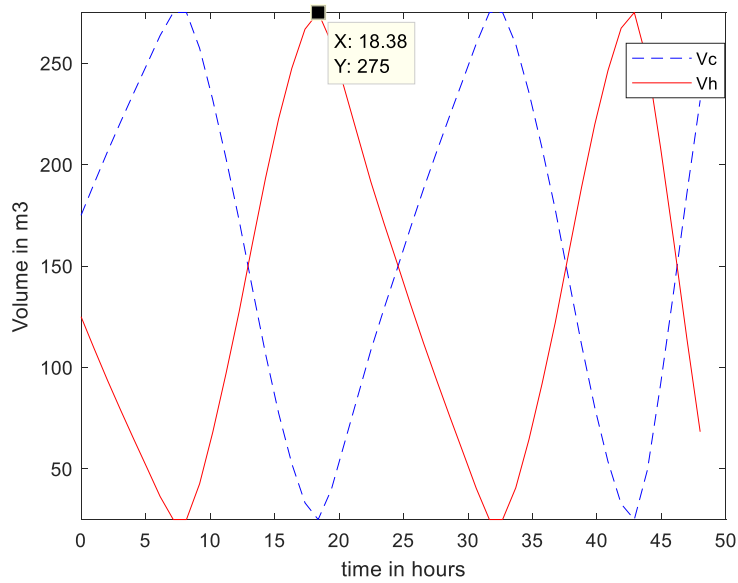


Figure 3-7 : Realistic case – TES tank volume profile

Similarly, we see from Figure 3-8 that the entire available duty from the supplier cannot be transferred and there is still dependence on external cooling and heating utilities as described in the earlier case.

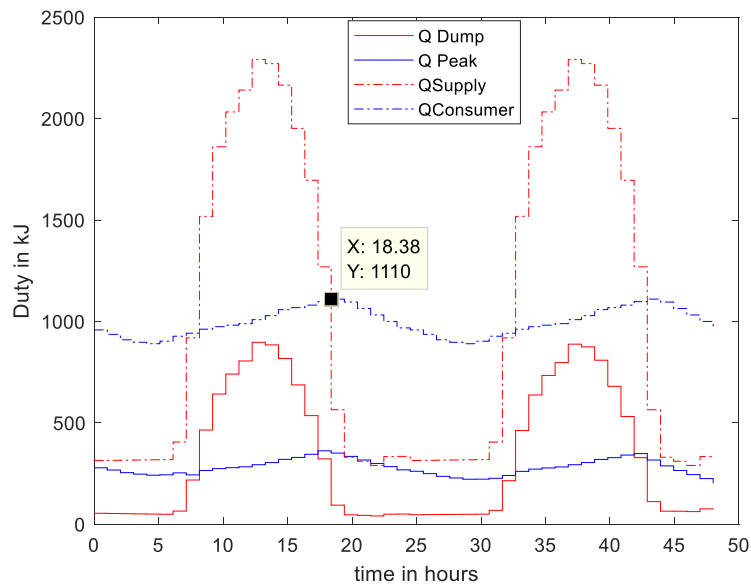


Figure 3-8 : Realistic case - External utilities usage profile

3.4. Discussion and Further Improvements

In Part 1 of this work, we have tried to address the Operations problem for a TES system with a nonlinear model and by solving an Optimal Control Problem to arrive at an optimal input trajectory. We could extend this work further to better align ourselves with the goal of integrating intermittent renewable sources of energy into the electricity grid by,

Optimal Control Under Uncertainties

Currently we have solved the control problem assuming perfect information of the future supply and demand profiles. These forecasts of future profiles are never known with certainty and even more important when we deal with renewables which are even more dependant on future weather conditions. Hence we could include implement the solution in a closed loop fashion with a Robust or Stochastic formulation of the MPC (depending on our tolerance to any constraint violations). Our problem is well suited for a Multistage Scenario based formulation, which is considered to be a more promising alternative for dynamic optimization under uncertainty [11].

Linking TES to Electricity Markets

Our current formulation is tailored to a case of thermally integrating process plants in an industrial cluster with TES as an intermediary. External utilities are imported to satisfy the demands and the objective was to minimize total cost of imported utilities. We could extend this system to link the TES to the electricity markets and participate in arbitrage based on uncertainty information of future demand and supply.

Part 2

Design Problem

Chapter 4. Optmal Design Problem

In the previous section, we saw the case of optimal operation without any uncertainties present. The Volume of the TES Tanks (V_{h_max} and V_{c_max}) and the area of the heat exchangers transferring heat to/ from the TES were fixed and assumed to be given. These parameters are chosen during the design of the plant and affect the operation of the TES plant. In this section, we focus on how these parameters are chosen by the designers. We first start with a simplified case of optimal design without any uncertainty and will extend the problem to handle uncertainties in the next chapter.

A simple objective function for the designer can be described to minimize the total cost during the lifetime of the plan for a fixed production profile. The costs manly can be split as initial Capital costs (C_{CAPEX}) and total Lifetime Operating costs (C_{OPEX}) which represents the total operating cost for the lifetime of the plant. Armed with a basic operating profile of the plant for the design life, the objective for the optimal design problem can be thus stated as

$$\min_{x_{opex} x_{capex}} C_{CAPEX} + C_{OPEX} \quad (4.1)$$

Where the x_{capex} represents variables chosen by the designer (in our example - the volume of the tank and exchanger area) and x_{opex} represents all the variables chosen for optimal operation (in our example - the TES flows and import of external utilities). Typically, the design life of chemical plants can be 20 years or more. These are highly simplifying assumptions and actual costing and project evaluation will account for inflation and other discounting factors to represent the net present value of costs, which we have ignored for simplicity.

We would be tempted to use the operations model developed in the previous section and including the design parameters also as variables while including the capital costs term into the objective of the OCP. Since the design problem is simulated for the entire design life of the plant, solving the nonlinear optimal control problem directly becomes somputationaly intractable.

We explore the option of developing a simplified linear Design model which can be effectively solved for the entire design life in this report.

4.1. Design Model

We formulate a simplified model based on duties for the TES system as shown in Figure 4-1.

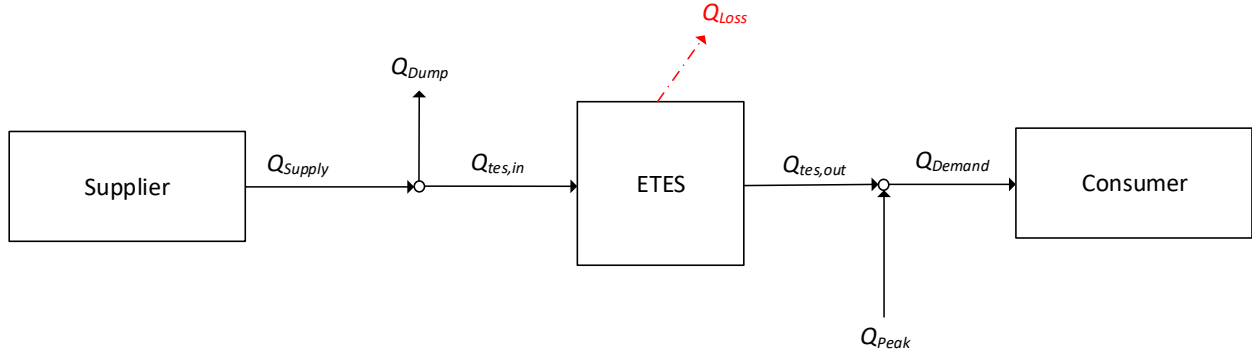


Figure 4-1: Design Model

Similar to the earlier case, we have the Supplier, which has the need to remove a given duty Q_{Supply} which is achieved by transferring to the TES ($Q_{tes,in}$) or rejected using a cold utility (Q_{Dump}). The consumer has a given duty demand (Q_{Demand}) which can be satisfied by energy from the TES ($Q_{tes,out}$) or by an eternal hot utility (Q_{Peak}). The charge of the TES is represented as E_{tes} which must be below the maximum capacity of the TES denoted as CAP_{tes} . The rate of heat transferred to/ from the TES is limited by the maximum power of the TES, denoted as POW_{tes} . The design parameters of interest in the actual TES plant (Volume of the TES tank and the Area of the heat exchangers) are represented using CAP_{tes} and POW_{tes} in the simplified linear model. The relationship between the design parameters for the actual TES and the simplified design model is described in more detail below.

Linking CAP_{tes} and Tank Volume ($V_{tes,max}$)

The maximum energy stored in the TES system depends on the total enthalpy change of the TES fluid between full charged and fully discharged states. From the two tank TES model, we can see this equals $CAP_{tes} = \rho_{tes} V_{tes} C_{p,tes} \Delta T$ where ΔT is the operating temperature window.

Considering ΔT to be 20 Deg C and property values for water, we get the relationship between the Volume and the Capacity of TES in the design model as,

$$V_{tes}^{(m^3)} = 43.06 CAP_{tes}^{(MWh)} \quad (4.2)$$

Linking POW_{tes} and Area of Exchangers

The maximum power rating POW_{tes} corresponds to the maximum duty transferred across the heat exchanger to/ from the TES given by $Q = UA_{Hex} \Delta T_{LMTD}$. The ability of the heat exchanger to transfer energy thus depends on the ΔT_{LMTD} which depends on the Temperatures of the hot and cold streams around the heat exchanger. These temperatures in turn depend on the flowrate of the hot and cold side streams in the heat exchanger as shown in Chapter 2. Hence, we cannot find a direct relationship between the heat exchanger area without accounting for the flowrates which are not considering in the design model. We can instead find an upper estimate of area required, which occurs when the driving force is at its minimum. It is standard engineering practice to take the lowest approach temperature in an exchanger to be between 10-15 Degrees during design. We consider the lowest approach temperature here as 15 Degrees, and the lowest LMTD then (occurs when the hot and cold Temperature profiles are parallel to each other) is 15 Degree C. Substituting properties for water, we can then find the relationship between Area of the exchanger and Power of TES in the design model as,

$$A_{Hex}^{(m^2)} = 60.24 POW_{tes}^{(MW)} \quad (4.3)$$

We can read this equation as, the maximum energy that an exchanger of area 60.24 m² can transfer is 1 MW. During operations however, higher driving forces are available by increasing the TES flow and the exchanger would be able to deliver more than this limit. We take the highly conservative approach of assuming this limit as the maximum power constraint for the TES in the design problem formulation. In the operations case such a limit would translates to artificially restricting flow of q_c/q_h to limit the transfer of energy to/ from the TES less than POW_{tes} . This is a highly conservative approach for operations which is being considered during design and the resultant area of exchanger arrived at from design would be much higher than needed for optimal operation.

Estimating Capital Cost (C_{CAPEX}) and Operating cost (C_{OPEX})

The operating cost is assumed similar to the operations problem with a linear cost model on usage of external utilities with costs $c_{peak}(t)$ and $c_{dump}(t)$. But since we define C_{OPEX} as the operating cost for the entire lifetime of the plant, we have

$$C_{OPEX} = \sum_{t=0}^N c_{peak} Q_{Peak}(t) + c_{dump} Q_{Dump}(t) \quad (4.4)$$

which is summed over the design life of the plant, typically in years.

We linearize the total purchased equipment cost curves as provided by Sinnott and Towler in [16], so that our problem can retain the linear form, and hence we can make use of efficient LP solvers for solving the large problem being formulated. Following the factorial method for converting the total purchased cost to total capital cost for the tank and heat exchanger, we get the total investment as,

$$C_{CAPEX}^{(USD_{2017})} = (82767 + 12875 CAP_{tes}) + (11184 + 35490 POW_{tes}) \quad (4.5)$$

The exact details of the purchased equipment cost curves and the factorial method for capital cost estimation used in this case are provided in Appendix A2.a.

4.2. Optimal Design without Uncertainty

We start the optimal design problem under the simple case where the future profile is perfectly known. Then the optimal design problem can be written down as,

$$\min_{x_{opex} x_{capex}} C_{CAPEX} + C_{OPEX} \quad (4.6.a)$$

$$\text{s.t. } CAP_{tes} \geq 0 \quad (4.6.b)$$

$$POW_{tes} \geq 0 \quad (4.6.c)$$

$$\dot{E}_{tes}(t) = Q_{tes}^{in}(t) - Q_{tes}^{out}(t) - Q_{loss}(t) \quad (4.6.d)$$

$$0 \leq Q_{Peak}(t) \leq Q_{Peak,max} \quad (4.6.e)$$

$$0 \leq Q_{Dump}(t) \leq Q_{Dump,max} \quad (4.6.f)$$

$$0 \leq Q_{tes}^{in}(t) \leq POW_{tes} \quad (4.6.g)$$

$$0 \leq Q_{tes}^{out}(t) \leq POW_{tes} \quad (4.6.h)$$

$$0 \leq E_{tes}(t) \leq CAP_{tes} \quad (4.6.i)$$

Where C_{OPEX} and C_{CAPEX} are defined as in Equations (4.4) and (4.5). Variables are defined as,

$$x_{CAPEX} = [CAP_{tes} \quad POW_{tes}] \quad (4.6.j)$$

$$x_{opex}(t) = [Q_{Dump}(t) \quad Q_{Peak}(t) \quad E_{tes}(t)] \quad t = 1 \dots N \quad (4.6.k)$$

And the constraints represent the rate of change of energy stored in the TES from the energy balance from Figure 4-1 and corresponding limits on maximum Capacity and Power of the TES.

Illustrative Case

We define an illustrative example where the profile given for the 1 day as shown in Figure 4-2 is repeated for the design life of 20 years for the plant. The daily profile for Q_{Supply} is higher than the Q_{Demand} in first half of the day and lower in the next. The total Supply and Demand energy is chosen as equal for simplifying the discussion in this case. The reader is encouraged to take note that the duties chosen here are similar to the illustrative case for the operations problem in section 3.2 to enable a consistent comparison between Operations and Design cases.

With the current coefficients chosen, we see that the optimal design is for a TES system with $CAP_{tes} = 6$ MWh and $POW_{tes} = 2$ MW, as it is cheaper to have the initial capital investment rather than an increased operating cost for the design life of 20 years. Figure 4-3 shows the daily operation profile where excess energy is charged into the TES and discharged when the demand is higher. The optimal power rating is matched with the maximum supply rate as to drive the use of Q_{Dump} to zero.

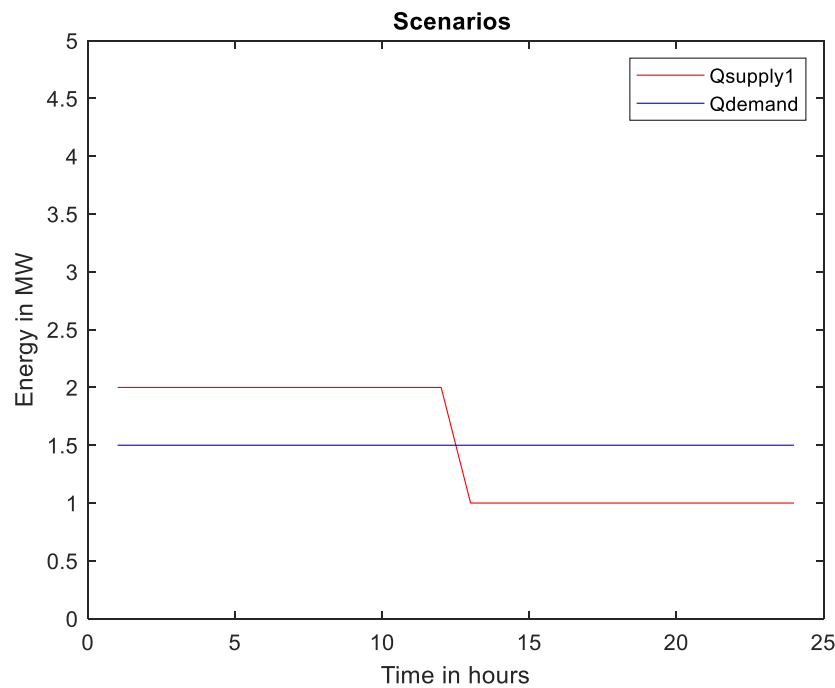


Figure 4-2 : Illustrative Design - Daily Profile (QSupply, QDemand)

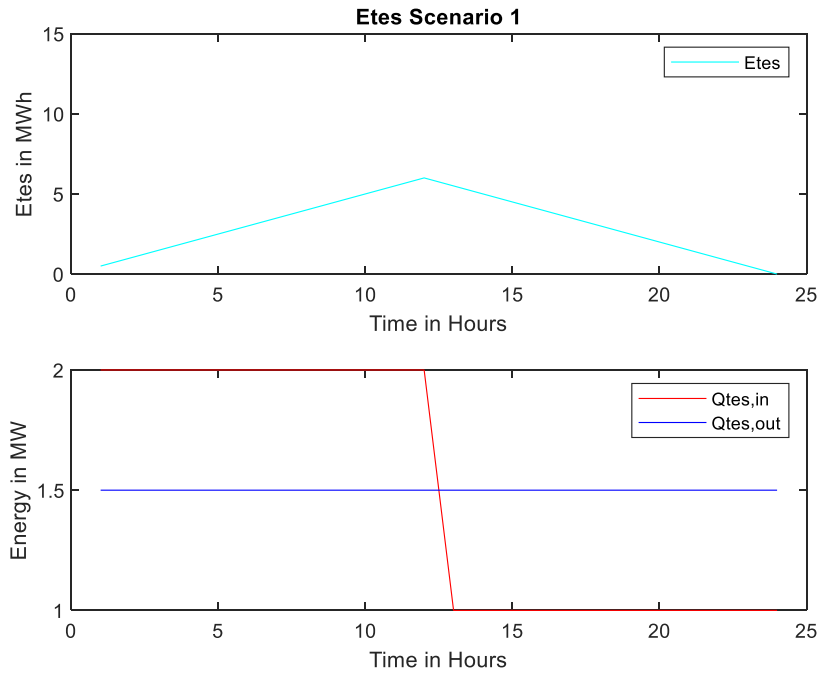


Figure 4-3 : Illustrative Design - TES Daily Operation

Chapter 5. Optimal Design Under Uncertainties

In this chapter we now expand the deterministic case from the previous chapter to handle uncertainties in the future profiles of Q_{Supply} and Q_{Demand} .

5.1. Two Stage Linear Stochastic Program with Recourse

We assume that information of future uncertainty is known and can be represented using a finite set of discrete scenarios. We do not explore the issues of scenario generation in this work, but assume that a finite set of scenarios S is provided, each with probability p_j where $\sum_{j \in S} p_j = 1$.

During actual operation of the plant a particular scenario would be realized, where we can take the operating variables in the linear design model as the recourse action for that scenario. This assumption is valid since during actual operations, we expect the corresponding input variables in the operations model (q_c, q_h and resultind Q_{Dump} and Q_{Peak}) to be manipulated by a closed loop implementation of the Optimal Control Problem we developed in Part 1 of this report (NMPC) to minimize the C_{OPEX} , if we do not expect uncertainty in the OCP horizon. In this case, our optimal design problem can be described as a two stage linear stochastic program with recourse. A classical two stage linear stochastic program with recourse is defined as

$$z^{SP} = \min_x c^\top x + \sum_{s=1}^S p_s Q_s(x) \quad (5.1.a)$$

$$\text{s.t. } Ax \geq b \quad (5.1.b)$$

$$x \in \mathbb{R}_+^{n_1} \quad (5.1.c)$$

where for $s = 1, \dots, S$

$$Q_s(x) \stackrel{\text{def}}{=} \min_{y_s} q_s^\top y_s \quad (5.1.d)$$

$$\text{s.t. } W_s y_s = h_s - T_s x \quad (5.1.e)$$

$$y_s \in \mathbb{R}_+^{n_2} \quad (5.1.f)$$

Here the vector x represents the first stage decision variable which are decisions that need to be taken without full information of some random variable. In our case, it represents the design decisions of CAP_{tes} and POW_{tes} we need to take without full information of which scenario is going to be realized during operation of the plant. In the second stage, for a given realization s ,

the second stage problem data q_s , W_s , h_s and T_s becomes known. In our case, the problem is of fixed recourse form since W_s is the constant for all scenarios. The second stage variables y_s are chosen such that the second stage objective function (5.1.d) is minimized subject to the second stage constraints (5.1.e) and (5.1.f). We wish to highlight the fact that there is only a single value for the first stage variable x , but each scenario has its corresponding second stage recourse variable y_s . The reader is directed to Chapters 1 and 3 in [17] for a more extensive discussion of the Two stage linear Stochastic Programs.

5.2. TES Design Problem under uncertainty

We can write our optimal design problem in the two stage linear stochastic program with fixed recourse as,

$$\min_{x_{\text{opex}}, x_{\text{capex}}} C_{\text{CAPEX}} + \sum_{s=1}^S p_s C_{\text{OPEX},s} \quad (5.2.a)$$

$$\text{s.t. } CAP_{\text{tes}} \geq 0 \quad (5.2.b)$$

$$POW_{\text{tes}} \geq 0 \quad (5.2.c)$$

$$\dot{E}_{\text{tes},s}(t) = Q_{\text{tes},s}^{\text{in}}(t) - Q_{\text{tes},s}^{\text{out}}(t) - Q_{\text{loss},s}(t) \quad (5.2.d)$$

$$0 \leq Q_{\text{Peak},s}(t) \leq Q_{\text{Peak,max}} \quad s = 1, \dots, S \quad (5.2.e)$$

$$0 \leq Q_{\text{Dump},s}(t) \leq Q_{\text{Dump,max}} \quad s = 1, \dots, S \quad (5.2.f)$$

$$0 \leq Q_{\text{tes},s}^{\text{in}}(t) \leq POW_{\text{tes}} \quad s = 1, \dots, S \quad (5.2.g)$$

$$0 \leq Q_{\text{tes},s}^{\text{out}}(t) \leq POW_{\text{tes}} \quad s = 1, \dots, S \quad (5.2.h)$$

$$0 \leq E_{\text{tes},s}(t) \leq CAP_{\text{tes}} \quad s = 1, \dots, S \quad (5.2.i)$$

Where C_{CAPEX} and C_{OPEX} are as defined in Equations (4.4) and (4.4). We employ a forward euler scheme to discretize the energy balance equation (5.2.d). We demonstrate the problem with an illustrative example below.

Optimal Design : Illustrative Case

Let us consider a simple example where there are 2 scenarios where the daily profiles for Q_{Supply} and Q_{Demand} are as given in Figure 5-1 and is assumed to repeat daily for the design life of 5 years of the plant. Let's consider scenario 1 is the most probable with $p_1 = 0.99$ and scenario 2 with $p_2 = 0.01$. In both scenarios, we consider total supply and demand is equal to keep the discussions simple. We can see that scenario 2 has a higher variation in the Supply profile.

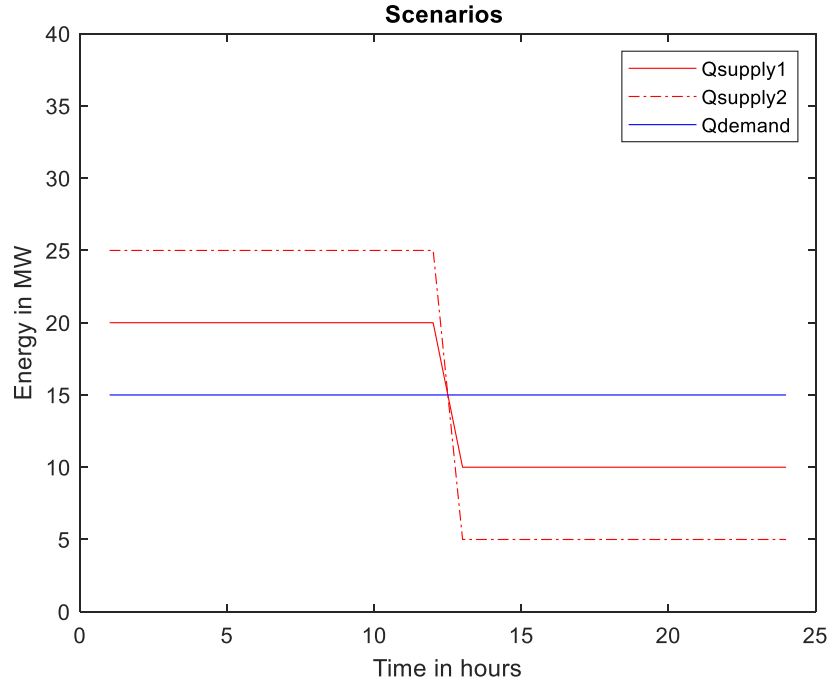


Figure 5-1 : Illustrative Stochastic Design - Daily Profile (QSupply, QDemand)

The optimal design for a deterministic case with only scenario 1 is $x_{capex} = [60 \ 20]$. Similarly, the optimal design for a deterministic case with only scenario 2 would be $x_{capex} = [120 \ 25]$, which needs a larger COP_{tes} and POW_{tes} due to the larger variation in the Supply profile. In the stochastic solution, we are trying to minimize sum of C_{CAPEX} and the expected value of the C_{OPEX} . We see the stochastic solution in this case is $x_{capex} = [60 \ 20]$ which will be a suboptimal choice if scenario 2 would be realized. This is due to the fact that the additional CAPEX of building a larger tank would be larger than the reduction in the expected OPEX for scenario 2. Hence $x_{capex} = [60 \ 20]$ is the optimal solution which minimizes the expected lifetime cost of the plant. The operation of the tank in case of both scenarios for the stochastic solution is shown in Figure 5-2. When scenario 2 is realized, since the tank is insufficiently sized, and it can be seen to be fully discharged at hour 19.

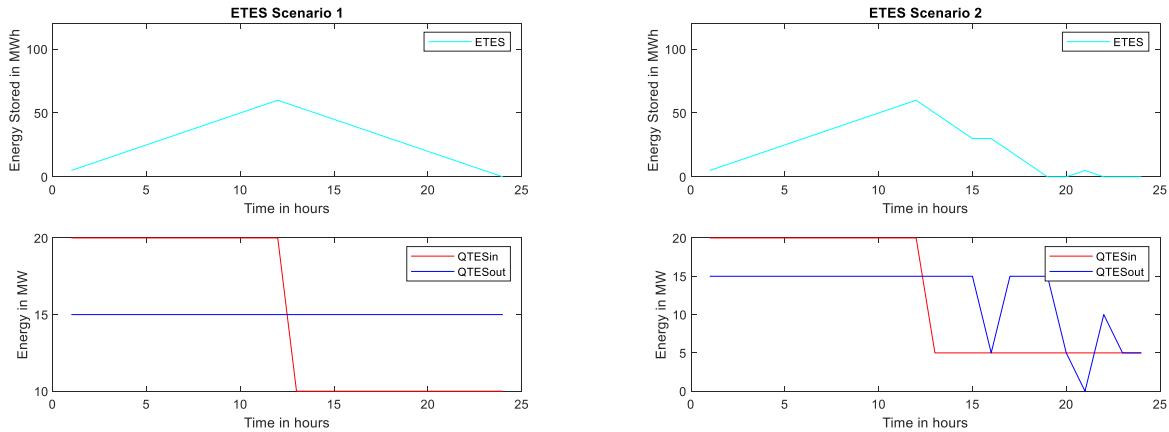


Figure 5-2 : Illustrative Stochastic Design - TES Daily Operation

The solution does seem trivial in this case, but in a real case where there are multiple scenarios with non-trivial probabilities provided, the two-stage formulation provides us the optimal decision to take with the known information of uncertainty.

We demonstrate this case with an application of this approach to the design of a TES system using scenarios generated from the data set from a district heating plant in northern Norway.

Optimal Design : Industrial Case

An industrial TES system with one supplier and one consumer as described in Section 4.1 is considered. Hourly data for the year of 2017 was obtained for a district heating company in Northern Norway, from which we extract equivalent profiles for Q_{Supply} and Q_{Demand} to our TES design model and is plotted in Figure 5-3. We can see that there is a seasonal variation in the thermal demand with lower heating demands during summer months while the supply of thermal energy is nearly stable.

During the winter months, the Supply and Demand profiles frequently cross each other and the installation of a TES system would help reduce the dependence on external utilities. A representative profile for a winter week is shown in Figure 5-4, and we can see that a TES would be able to charge during periods of excess supply and dispatch it during periods of shortfall, thus reducing import of electricity.

There are also variations in the electricity prices as shown in Figure 5-4, and a TES would be able to take advantage of storing energy during periods of low electricity prices and dispatch it

during periods of higher electricity prices to minimize the operating costs. Since no information was available, the prices for heat dumping is considered to be $1/10^{\text{th}}$ of the peak heating prices.

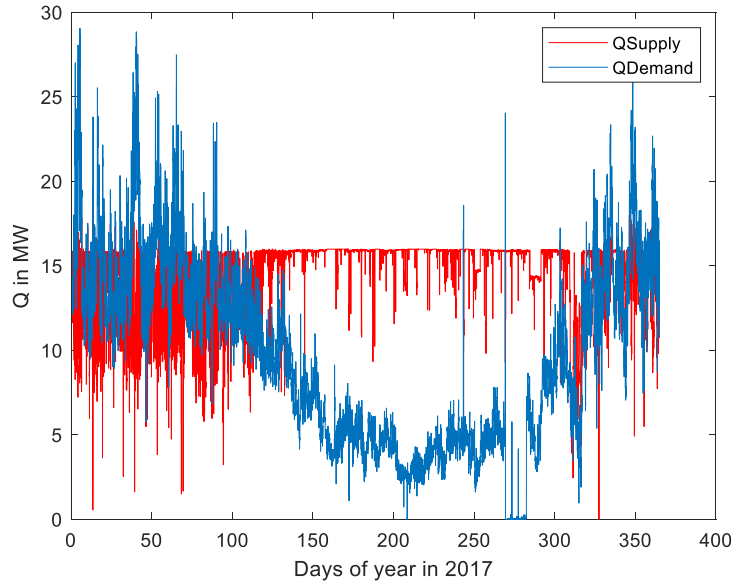


Figure 5-3 : Indutry Year Data

We consider 13 representative scenarios to account for the uncertainty in profiles for Q_{Supply} , Q_{Demand} and Q_{Peak_cost} , in which the weekly profiles are assumed to repeat for the design life of 5 years. The adequacy of these scenarios to represent the reality is not considered in detail here, as scenario generation is not the main focus of our study. Assuming equal probability for each scenario, arriving at the optimal design decision is not a trivial task, and hence demonstrates the usefulness of the stochastic formulation we developed.

The solution for the Stochastic problem gives us the maximum capacity and power of the required TES as $x_{capex} = [92.2 \quad 21.83]$. The Optimal recourse actions in the case of Scenario 5 is shown in Figure 5-5 and Figure 5-6. We can also see that it is optimal at times to conserve the charge in the TES during periods of low electricity prices and later dispatch it during periods of higher electricity prices, as is the case in day 5 in Figure 5-6.

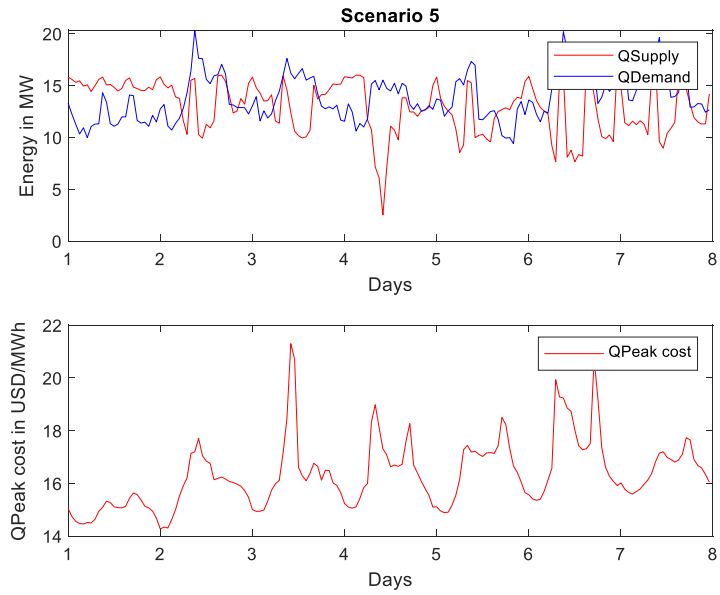


Figure 5-4 : Representative Weekly data – Supply and Demand Profiles

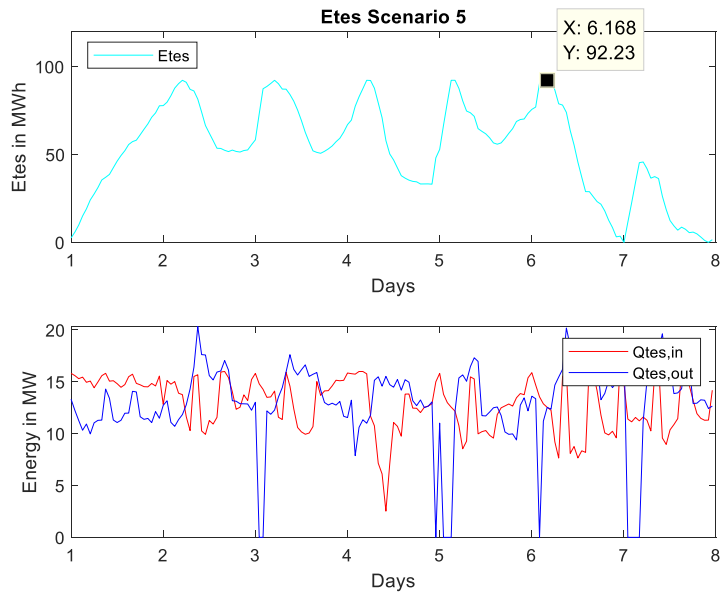


Figure 5-5 : Recourse Action for scenario 5

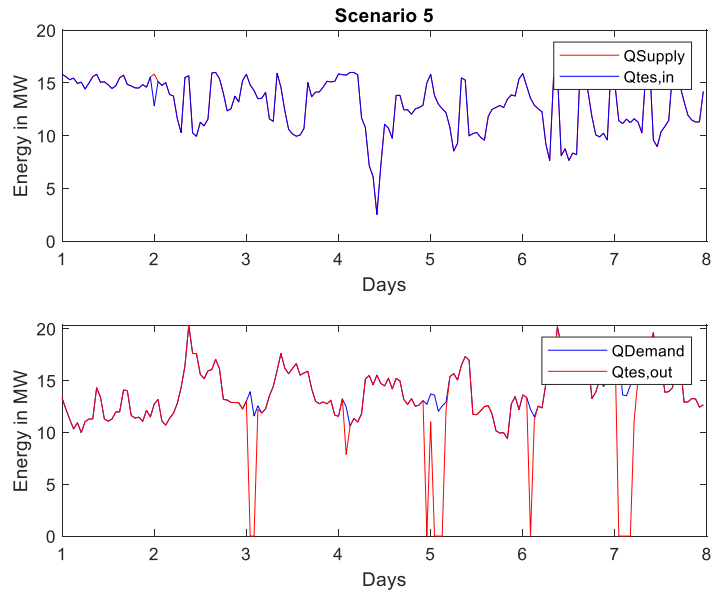


Figure 5-6 : Recourse Action for scenario 5

5.3. Discussion and Further Improvements

In Part 2 of this work, we have tried to address the design problem for a TES System with a linear approximation of the actual design problem assuming a finite set of scenarios are provided which represent the uncertainty in parameters. This approach could be further improved by attention along the following major areas,

Selection of Scenarios

Currently we have assumed that the set of scenarios are given to us, and not much focus was put on ensuring that these scenarios do accurately represent the uncertainties. We could employ Monte Carlo based sampling methods or other data driven methods to build the representative scenario set when historical data is available as reference, ensuring that the number of scenarios do not increase exponentially with the number of uncertain parameters.

Relaxing linear approximations in Objective Function

Our current formulation of the objective function consists of linear approximation of the Capital cost estimation. We could relax this linear approximation with more representative costing relationships available in literature if we allow the objective function to be nonlinear. We could

also quickly account future operating costs in the objective with their Net Present Values to have a more realistic representation of the decision making process that is considered during design.

Relaxing the linear approximations in the Model

The current attempt at developing the linear approximation for the nonlinear process gives us an upper limit for the exchanger area required. If we could formulate and solve the design problem in terms of flows and temperatures, we can arrive at an exact solution. But as discussed in Chapter 4, the introduction of Temperatures and Flows make the model nonlinear and solution of this problem for the required time scales for design becomes computationally intractable. We could explore efficient decomposition strategies to reduce the computational effort or even reformulate the problem in a block separable form with only minor deviations from the optimal solution in future work.

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Appendix

A1. Two Tank TES Model

A1.a. Cell Model Approximation of Heat Exchangers

The Cell model approximation for modelling the heat exchangers is presented here,

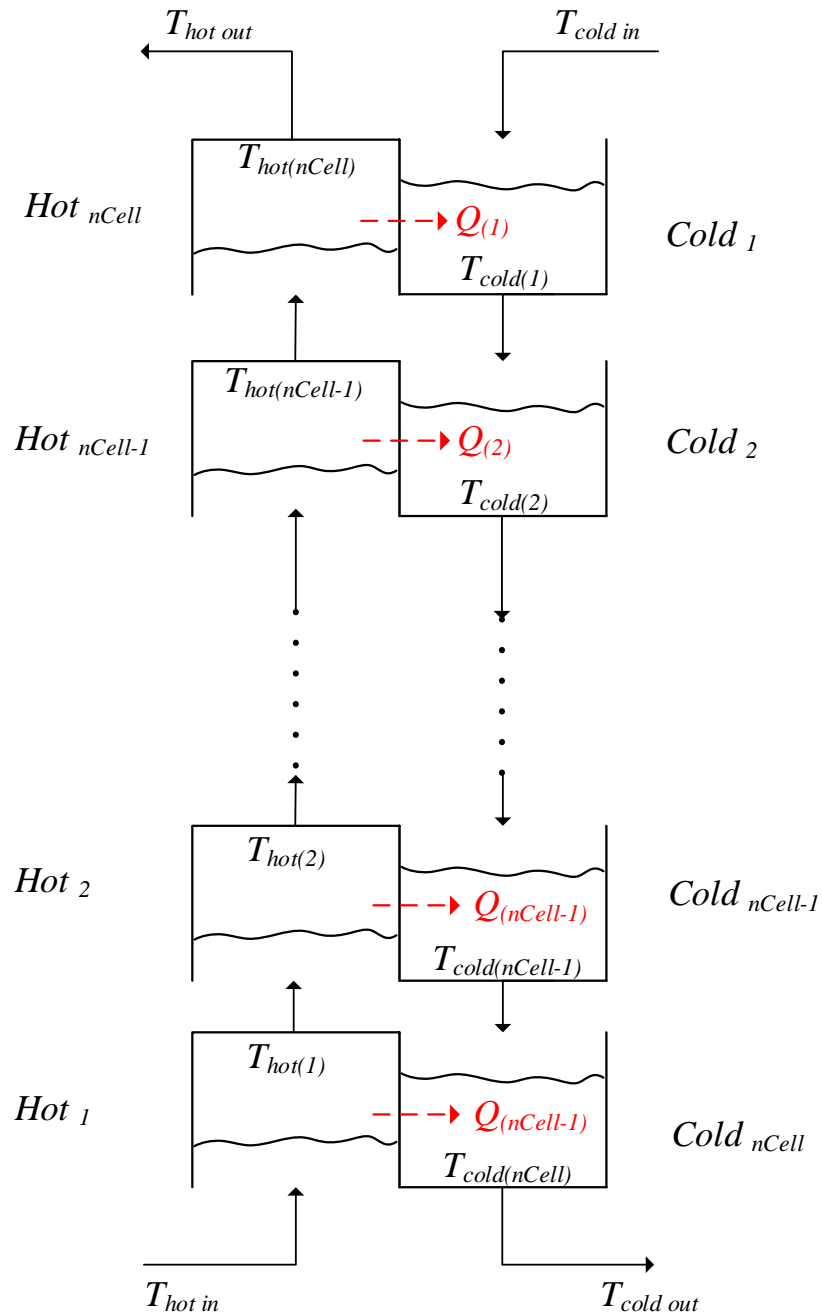


Figure A 1-1: Cell model approximation for modelling Heat Exchanger

The Hot stream enters from the bottom while the Cold from the top and numbered from entry to exit. The total Area and volume of the exchanger tube and shell sides are equally distributed among the $nCells$. The exit temperature of the exchanger is the temperature of the last cell and hence the Hot and Cold exit temperatures from the exchanger is referenced as $T_{Hot(nCell)}$ and $T_{Cold(nCell)}$.

The duty transferred from the hot side to the cold side in the k^{th} Cell can be calculated as

$$Q_k = hA_{Cell} (T_{hot(nCell+1-k)} - T_{cold(k)}) \quad k = 1, \dots, nCell \quad (A1.1)$$

Therefore, the change of temperature in the k^{th} Cell can be written as

$$\frac{dT_{cold(k)}}{dt} = \frac{hA (T_{hot(nCell+1-k)} - T_{cold(k)})}{\rho_{cold} V_{Cell(k)} C_{P_cold}} \quad k = 1, \dots, nCell \quad (A1.2)$$

$$-\frac{dT_{hot(nCell+1-k)}}{dt} = \frac{hA (T_{hot(nCell+1-k)} - T_{cold(k)})}{\rho_{hot} V_{Cell(nCell+1-k)} C_{P_hot}} \quad k = 1, \dots, nCell \quad (A1.3)$$

A1.b. Mass and Energy Balances

With the approximation of Heat Exchangers as Cells with $nCell = 3$, we can write the mass and Energy balance equations for

Energy Balance equations in Hex_Sup

For the k^{th} Cell element ($k = 1, \dots, nCell$), we have

$$\frac{d(\rho_{Sup} V_{Cell} C_{P_Sup} T_{Sup_e(k)})}{dt} = \frac{q_{Sup}}{3600} \rho_{Sup} C_{P_Sup} (T_{Sup_e(k-1)} - T_{Sup_e(k)}) - Q_{(k)} \quad (A1.4)$$

$$\frac{d(\rho_c V_{Cell} C_{P_c} T_{c_e(k)})}{dt} = \frac{q_c}{3600} \rho_c C_{P_c} (T_{c_e(k-1)} - T_{c_e(k)}) + Q_{(k)} \quad (A1.5)$$

Where $T_{Sup_e(0)}$ is T_{Sup_s} and $T_{c_e(0)}$ is T_c

Energy Balance equations in Hex_Con

For the k^{th} Cell element ($k = 1, \dots, nCell$), we have

$$\frac{d(\rho_h V_{Cell} C_{P_h} T_{h_e(k)})}{dt} = \frac{q_h}{3600} \rho_h C_{P_h} (T_{h_e(k-1)} - T_{h_e(k)}) - Q_k \quad (A1.6)$$

$$\frac{d(\rho_{Con} V_{Cell} C_{P_Con} T_{Con_e(k)})}{dt} = \frac{q_{Con}}{3600} \rho_{Con} C_{P_Con} (T_{Con_e(k-1)} - T_{Con_e(k)}) + Q_k \quad (A1.7)$$

Where $T_{h_e(0)}$ is T_h and $T_{Con_e(0)}$ is T_{Con_s}

Mass and Energy Balance across the storage tanks

$$\frac{dV_c}{dt} = \frac{q_h}{3600} - \frac{q_c}{3600} \quad (A1.8)$$

$$\frac{dV_h}{dt} = \frac{q_c}{3600} - \frac{q_h}{3600} \quad (A1.9)$$

$$\frac{d(\rho_{TES} V_c C_{p_TES} T_c)}{dt} = \rho_{TES} C_{p_TES} \left(\frac{q_h}{3600} T_{h_e} - \frac{q_c}{3600} T_c \right) \quad (A1.10)$$

$$\frac{d(\rho_{TES} V_h C_{p_TES} T_h)}{dt} = \rho_{TES} C_{p_TES} \left(\frac{q_c}{3600} T_{c_e} - \frac{q_h}{3600} T_h \right) - Q_{loss_h} \quad (A1.11)$$

Where the heat loss from the hot tank is defined as

$$Q_{loss_h} = U_{hot_tank} A_{hot_tank} (T_h - T_{amb}) \quad (A1.12)$$

With the assumptions of perfect mixing and combining equations, we get the ODE's for the model in Section Model Equations.

A1.c. Model Parameters

The constant parameters used in the Two Tank TES Model is defined in the parameters.m file, attached in Appendix A3.a below.

A2. Design Model

A2.a. Capital Cost Estimation

The Total Fixed Capital Cost is estimated using the factorial method as described in Towler and Sinnott [16]. The total purchase cost was estimated using correlation of the form,

$$C_e = a + bS^n \quad (\text{A2.1})$$

Where C_e represents the Purchased Equipment Cost in U.S. Gulf Coast basis, January 2006 and S is the size parameter for the equipment. The parameters as provided for

- Storage Tanks : Cone Roof

S = Volume	Value	Units	Coefficients	Value
High limit	10	m ³	a	5700
Low Limit	8000	m ³	b	700
			n	0.7

Table A2-1 : Tank Purchased Cost parameters

- Heat Exchanger : U-tube shell and tube

S = Area	Value	Units	Coefficients	Value
High limit	10	m ²	a	10000
Low Limit	1000	m ²	b	88
			n	1

Table A2-2 : Exchanger Purchased Cost parameters

Since it can be seen from Figure A2-1 and Figure A2-2, the equipment purchased cost is fairly linear at the range of capacities of interest, we use a linear best fit to estimate the Purchase cost from the capacities.

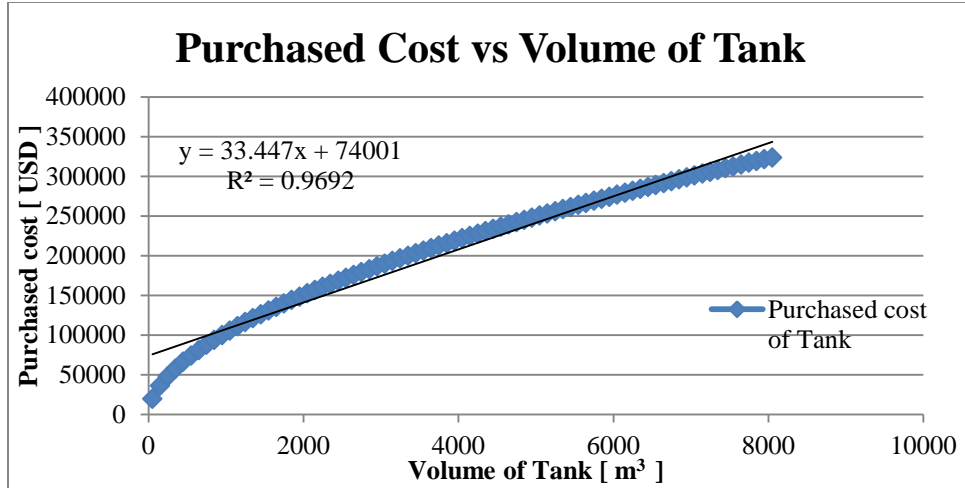


Figure A2-1 : Purchased cost relationship with Tank Volume

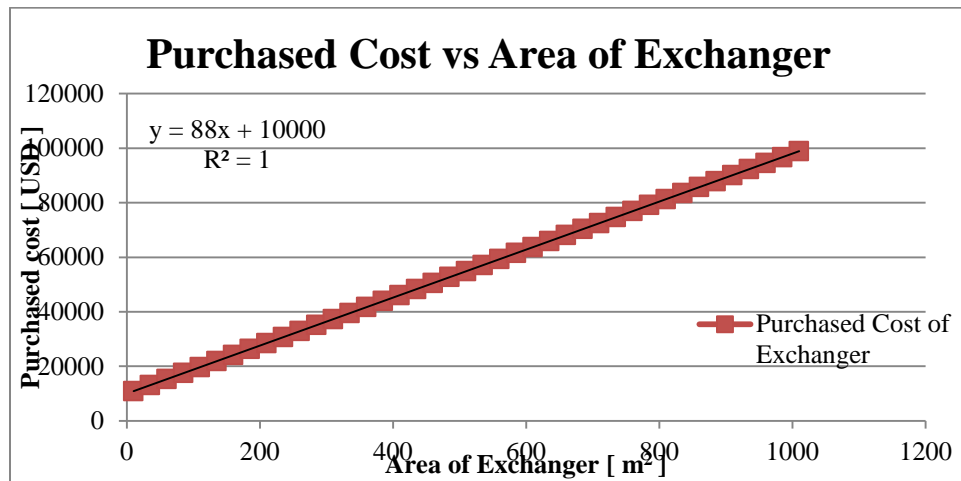


Figure A2-2 : Purchased cost relationship with Heat Exchanger Area

$$C_{\text{Tank}}^{(\text{USD}_{2006})} = (74001 + 33.4\text{Vol}^{m^3}) \quad (\text{A2.2})$$

$$C_{\text{Hex}}^{(\text{USD}_{2006})} = (10000 + 88\text{Area}^{m^2}) \quad (\text{A2.3})$$

The Project fixed Capital cost was estimated from the equipment purchase cost using the combined installation factor of 6 recommended for process type of Fluids in [16]. The Capital cost data since was available with the basis of 2006 (CEPCI 478.6) , was scaled to 2018 values (CEPCI 605.2) using the Chemical Engineering Plant Cost index.

$$\text{Cost in year A} = \text{Cost in year B} \frac{\text{Cost index in year A}}{\text{Cost index in year B}} \quad (\text{A2.4})$$

A3. Source Codes – Operations Model

A3.a. Parameters.m

Defenition of all constant parameters used,

```
global nCSTR;

%Supply parameters
Tsup_s = 100;      % Deg C
Tsup_r = 40;      % Deg C
rho_sup = 1000;   % kg/m3
CP_sup = 3.05558; % Supplier CP (taken as Thermic fluid)
Vhe_sup = 1;      % Supply side Heat exchanger volume
hAsup = 1*150/(nCSTR*2); % Supply Heat exchanger hA

% Consumer parameters
Tcon_s = 10;      % Deg C
Tcon_r = 70;      % Deg C
rho_con = 1000;   % kg/m3
CP_con = 3.05558; % Consumer CP (taken as Thermic fluid)
Vhe_con = 1;      % Supply side Heat exchanger volume
hAcon = 1*150/(nCSTR*2); % Consumer Heat exchanger hA

% TES Parameters
rho_t = 1000;     % Density of TES medium (kg/m3)
CP_t = 4.18;     % CP of TES medium
Vhe_c = 1;       % Cold side Heat exchanger volume (m3)
Vhe_h = 1;       % Hot side Heat exchanger volume (m3)

Vh_max = 275;    % Maximum hot tank volume (m3)
Vc_max = 275;    % Maximum cold tank volume (m3)
Vh_min = 25;     % Minimum hot tank volume (m3)
Vc_min = 25;     % Minimum cold tank volume (m3)

vdot_cold_min = 1; % Minimum cold flow (m3/hr)
vdot_hot_min = 1; % Minimum hot flow (m3/hr)
vdot_cold_max = 100; % Maximum cold flow (m3/hr)
vdot_hot_max = 100; % Maximum cold flow (m3/hr)

% Common Parameters
Tamb = 20;
UAh = 0; % Heat loss coefficient of hot tank
UAc = 0; % Heatloss coefficient of cold tank
```

A3.b. Model_dot.m

Model equations for state evolution,

```
% Ordinary Differential Eqns
Thot_in = Tsup_s;
Tcold_in = Tc;
for i=1:nCSTR
    x1dot{i} = ((vdot_sup/(3600*Vhe_sup/nCSTR))*(Thot_in-Tsup_e(i))-
(Qsup(i)/(Vhe_sup/nCSTR*rho_sup*CP_sup)));
    Thot_in = Tsup_e(i);
```

```

        x4dot{i} = ((vdot_cold/(3600*Vhe_c/nCSTR))*(Tcold_in-Tc_e(i))+(Qsup(nCSTR+1-
i)/(Vhe_c/nCSTR*rho_t*CP_t)));
        Tcold_in = Tc_e(i);
    end

    Thot_in = Th;
    Tcold_in = Tcon_s;
    for i=1:nCSTR
        x5dot{i} = ((vdot_hot/(3600*Vhe_h/nCSTR))*(Thot_in-Th_e(i))-
(Qcon(i)/(Vhe_h/nCSTR*rho_t*CP_t)));
        Thot_in = Th_e(i);

        x6dot{i} = ((vdot_con/(3600*Vhe_con/nCSTR))*(Tcold_in-
Tcon_e(i))+(Qcon(nCSTR+1-i)/(Vhe_con/nCSTR*rho_con*CP_con)));
        Tcold_in = Tcon_e(i);
    end

    x2dot = ((vdot_hot/(3600*Vc))*(Th_e(nCSTR)-Tc)-(Qloss_c/(Vc*rho_t*CP_t)));
    x3dot = ((vdot_cold/(3600*Vh))*(Tc_e(nCSTR)-Th)-(Qloss_h/(Vh*rho_t*CP_t)));
    x7dot = (vdot_hot - vdot_cold)/3600;
    x8dot = (vdot_cold - vdot_hot)/3600;

    xdot =
[vertcat(x1dot{:});x2dot;x3dot;vertcat(x4dot{:});vertcat(x5dot{:});vertcat(x6dot{:});x
7dot;x8dot];
end

```

A3.c. Optimal_Control_Problem.m

Solving the Optimal Control Problem

```

clear;

close all;
import casadi.*

global nCSTR N
nCSTR = 3;      % # of discretizations for Heat Exchangers

T = 2*24*3600; % Time horizon (seconds)
N = 2*24;      % number of control intervals
dt = T/N;      %(seconds)

% Parameters
parameters    % Loading model Parameters from .m file

```

```

%% Declare Model Variables
offset = 1.0;

% States
x1 = MX.sym('x1',nCSTR);
x2 = MX.sym('x2');
x3 = MX.sym('x3');
x4 = MX.sym('x4',nCSTR);
x5 = MX.sym('x5',nCSTR);
x6 = MX.sym('x6',nCSTR);
x7 = MX.sym('x7');
x8 = MX.sym('x8');
x = [x1; x2; x3; x4; x5; x6; x7; x8];
% x0 = [100*ones(nCSTR,1); 30; 80; 70*ones(nCSTR,1); 30*ones(nCSTR,1);
20*ones(nCSTR,1); 125; 125];
    % x0 from steady state CSTR3 (optimal Steady state)
    x0 =
offset.*[81.6480241404674;68.7906188056782;59.7827129139836;47.0439037095066;62.956096
3332679;50.6079206442220;55.6950087389464;62.9560475282138;59.3920793954863;54.3049912
962709;47.0439525006192;28.3519758738163;41.2093812189759;50.2172871181283;(Vh_max+Vh_
min)/2;(Vh_max+Vh_min)/2];
x0_min = [Tcon_s*ones(nCSTR,1); Tcon_s; Tcon_s; Tcon_s*ones(nCSTR,1);
Tcon_s*ones(nCSTR,1); Tcon_s*ones(nCSTR,1); Vc_min; Vh_min];
x0_max = [Tsup_s*ones(4*nCSTR + 2,1); Vc_max; Vh_max];

% Inputs/ Manipulated Variables
u1 = MX.sym('u1');
u2 = MX.sym('u2');
u3 = MX.sym('u3');
u4 = MX.sym('u4');
u = [u1; u2; u3; u4];
% u0 = [1273.1583; 1273.1583; 4.3860; 4.3860];
    % u0 from steady state (optimal Steady state)
    u0 =
offset.*[503.731891660742;503.731891247240;55.4287516160681;55.4287516161166];
u0_min = [0.01; 0.01; vdot_cold_min; vdot_hot_min];
u0_max = [1e4; 1e4; vdot_cold_max; vdot_hot_max];

nx = 8+(nCSTR-1)*4;
nu = 4;
nz = 0;

%% Supplier and Consumer Profiles

    % Scaled Duck curve profile
    [vdot_supply, vdot_consumer] = ScaledProfile(N);
    vdot_consumer = 1.5.*vdot_consumer;
% Step change Profile
%     vdot_supply = [30*ones(N/2,1); 30*ones(N/2,1)]; % m3/hr
%     vdot_consumer = [30*ones(N/2,1); 30*ones(N/2,1)]; % m3/hr

```

```

% Plotting Supplier and Consumer flow profiles
tgrid = linspace(0, N, N);
figure
stairs(tgrid, vdot_supply, 'r');
hold on;
stairs(tgrid, vdot_consumer, 'b');
ylim([0 50]); xlabel('time in hours'); ylabel('Flow in m3/hr')
legend('vdot_supply','vdot_consumer' )

QDump_noTES = rho_sup*CP_sup*(Tsup_s-Tsup_r)/3600.*vdot_supply;
QPeak_noTES = rho_con*CP_con*(Tcon_r-Tcon_s)/3600.*vdot_consumer;

% Fixed Parameters (Passed as Casadi Variables)
% Used in Optimal SS and Integrator Defenition
vdot_sup = MX.sym('vdot_sup');
vdot_con = MX.sym('vdot_con');
vdot_p = [vdot_sup; vdot_con];
vdot_p0 = [vdot_supply(1);vdot_consumer(1)];

[xdot] = Model_dot(x, u, vdot_p);

% Objective term

L = u1 + u2;

% Finding Optimal steady state
% [x0, u0] = Optimal_SteadyState(x0, u0, vdot_p0 )

%% Integrator

% CVODES from the SUNDIALS suite
dae = struct('x',x,'p',[u;vdot_p],'ode',xdot,'quad',L);
opts = struct('tf',dt);
F = integrator('F', 'cvodes', dae, opts);

% Evaluate at a test point
Fk = F('x0',x0,'p',[u0;vdot_p0]);

% NLP

w={};

w0 = [];

lbw = [];

ubw = [];

```

```

J = 0;

g={};

lbg = [];

ubg = [];

% "Lift" initial conditions
Xk = MX.sym('X0', 4*nCSTR+4);
w = {w{:}, Xk};
lbw = [lbw; x0];
ubw = [ubw; x0];
w0 = [w0; x0];

% Formulate the NLP

for k=0:N-1
    % New NLP variable for control (MV's)
    Uk = MX.sym(['U_' num2str(k)],4);
    w = {w{:}, Uk};
    lbw = [lbw; u0_min];
    ubw = [ubw; u0_max];
    w0 = [w0; u0];

    % Integrate till the end of the interval
    Fk = F('x0',Xk,'p', [Uk; vdot_supply(k+1);vdot_consumer(k+1)]);

    Xk_end = Fk.xf;
    J=J+Fk.qf;

    % New NLP variable for state at end of interval
    Xk = MX.sym(['X_' num2str(k+1)], 4*nCSTR+4);
    w = [w, {Xk}];
    lbw = [lbw; x0_min];
    ubw = [ubw; x0_max];
    w0 = [w0; x0];

    % Add shooting gap -> State equality constraint
    g = {g{:}, Xk_end-Xk};
    lbg = [lbg; x0-x0];
    ubg = [ubg; x0-x0];

    % Additional constraints (approach temp in each CSTR)
    for i=1:nCSTR
        g = {g{:}, [(Xk(i)-Xk(2*nCSTR+3-i)), (Xk(2*nCSTR+2+i)-Xk(4*nCSTR+3-i))]'};
        lbg = [lbg; 0; 0];
        ubg = [ubg; inf; inf];
    end
end

```

```

    g = {g{:}, [ vdot_supply(k+1)/3600*rho_sup*CP_sup*(Tsup_r - Xk(nCSTR)) + Uk(1),
vdot_consumer(k+1)/3600*rho_con*CP_con*(Xk(4*nCSTR+2) - Tcon_r) + Uk(2) ]'};
    lbq = [lbq; [0 0]'];
    ubq = [ubq; [inf inf]'];

end
%% NLP Solver

opts = struct;

opts.ipopt.max_iter = 1000;

prob = struct('f', J, 'x', vertcat(w{:}), 'g', vertcat(g{:}));
solver = nlpso('solver', 'ipopt', prob,opts);

% Solve the NLP
sol = solver('x0', w0, 'lbx', lbw, 'ubx', ubw, ...
            'lbq', lbq, 'ubq', ubq);

w_opt = full(sol.x);
optcost = full(sol.f)
Cumul_cost0 = (u0(1) + u0(2))*T

%% Calculating Profiles for Plots

x_opt = [];

u_opt = [];

for k=0:N-1
    x_opt = [x_opt, w_opt( ((nx+nu+nz)*k+ 1) : ((nx+nu+nz)*k + nx) )];
    u_opt = [u_opt, w_opt( ((nx+nu+nz)*k+ nx+1) : ((nx+nu+nz)*k + nx+nu) )];
end

%% Plots
tgrid = linspace(0, N, N);

% Plotting State Profiles
% Plotting Temperatures
figure
plot(tgrid, x_opt(nCSTR,:), '--');
hold on;
plot(tgrid, x_opt(nCSTR+1,:), '-');
hold on;
plot(tgrid, x_opt(nCSTR+2,:), '-');
hold on;

```

```

plot(tgrid, x_opt(2*nCSTR+2,:), '-');
hold on;
plot(tgrid, x_opt(3*nCSTR+2,:), '-');
hold on;
plot(tgrid, x_opt(4*nCSTR+2,:), '-');
xlabel('time in hours'); ylabel('Temp in Deg C')
legend('Tsup_e', 'Tc', 'Th', 'Tc_e', 'Th_e', 'Tcon_e')
% Plotting Tank Levels
figure
plot(tgrid, x_opt(4*nCSTR+3,:), 'b--');
hold on;
plot(tgrid, x_opt(4*nCSTR+4,:), 'r-');
xlabel('time in hours'); ylabel('Volume in m3'); ylim([Vh_min Vh_max])
legend('Vc', 'Vh')

% Plotting MV's
% Plotting Utility Loads
figure
stairs(tgrid, u_opt(1,:), 'r')
hold on
stairs(tgrid, u_opt(2,:), 'b')
hold on
stairs(tgrid, QDump_noTES, 'r-.')
hold on;
stairs(tgrid, QPeak_noTES, 'b-.')
xlabel('time in hours'); ylabel('Duty in kJ');
legend('Q Dump', 'Q Peak', 'QSupply', 'QConsumer')
% Plotting TES Flows
figure
stairs(tgrid, u_opt(3,:), 'b-.')
hold on
stairs(tgrid, u_opt(4,:), 'r-.')
xlabel('time in hours'); ylabel('Flow in m3/hr'); ylim([vdot_hot_min vdot_hot_max]);
legend('q_c', 'q_h')

figure
plot(tgrid, x_opt(nCSTR,:), 'r');
hold on;
plot(tgrid, x_opt(nCSTR-1,:), 'r-.');
hold on;
plot(tgrid, x_opt(nCSTR-2,:), 'r:');
hold on
plot(tgrid, x_opt(2*nCSTR+2,:), 'b:');
hold on;
plot(tgrid, x_opt(2*nCSTR+2-1,:), 'b-.');
hold on;
plot(tgrid, x_opt(2*nCSTR+2-2,:), 'b');
hold on;

```



```

    xlabel('time in hours'); ylabel('Temperature in Deg C'); title('Supplier HEx
Profiles')
    legend('Tsup_e 3','2','1', '3','2','Tc_e 1')

figure
plot(tgrid, x_opt(3*nCSTR+2,:), 'r:');
hold on;
plot(tgrid, x_opt(3*nCSTR+2-1,:), 'r-.');
hold on;
plot(tgrid, x_opt(3*nCSTR+2-2,:), 'r');
hold on;
plot(tgrid, x_opt(4*nCSTR+2,:), 'b');
hold on;
plot(tgrid, x_opt(4*nCSTR+2-1,:), 'b-.');
hold on;
plot(tgrid, x_opt(4*nCSTR+2-2,:), 'b:');
hold on;
xlabel('time in hours'); ylabel('Temperature in Deg C'); title('Consumer HEx
Profiles')
legend('3','2','Th_e 1','Tcon_e 3','2','1')

```

A4. Source Codes – Design Model

A4.a. Parameters.m

Constant Parameters used in the model.

```
% CAPEX Coefficients
c1_eTES = 12875 ; % USD/(MWh) Unit cost of Tank Capacity
c1_pTES = 35490 ; % USD/(MW) Unit cost of Tank Power

c0_eTES = 82767 ; % USD/(MWh) Constant term for Tank cost
c0_pTES = 11184 ; % USD/(MW) Constant term for HEx cost

% Heat Loss from Tank
beta = 0 ; % Heat loss coefficient

% Max limits
eTES_max = inf ; %
pTES_max = inf ; %
QDump_max = inf ; %
QPeak_max = inf ; %

% Initial Conditions/ Guesses
eTES0 = 1 ; %
pTES0 = 1 ; %
```

A4.b. Two_Stage_Stochastic_Program.m

Solving the Two Stage Stochastic Problem in extensive form.

```
clear

close all;
import cplex.*

Day_sim = 1; % Length of each scenario in Days
NDays = 1; % Total Number of days in data file
Tsim = 24*Day_sim;
dt = 1;
N = Tsim/dt;
S = floor(NDays/Day_sim); % Number of Scenarios
prob_s = 1/S*ones(S,1);
% prob_s = [0.99; 0.01]
run_time = [];

% Import Parameters
```

```

parameters;

QSupply = zeros(N,S);
QDemand = zeros(N,S);

% Generate New Data
tic
[QSupply, QDemand, QDump_cost, QPeak_cost] = GenerateProfile(N, S);
t = toc;
run_time{1,1} = ['Generate Profile_', num2str(t)];

Days_plot = [linspace(1,24,24)',linspace(1,24,24)'];

%           % Save QDemand, QSupply, QPeak_cost to .mat file for later use
%           save('test24X5.mat','QDemand')
%           save('test24X5.mat','QSupply', '-append')
%           save('test24X5.mat','QPeak_cost', '-append')

QDump0 = 0;

QPeak0 = 0;

ETES0 = 0;

tic

TESprob = optimproblem;

%Declaring Variables
eTES = optimvar('eTES',1, 'LowerBound', 0, 'UpperBound', eTES_max);
pTES = optimvar('pTES',1, 'LowerBound', 0, 'UpperBound', pTES_max);

QDump = optimvar('QDump',N,S, 'LowerBound',0, 'UpperBound', QDump_max);
QPeak = optimvar('QPeak',N,S, 'LowerBound',0, 'UpperBound', QPeak_max);
ETES = optimvar('ETES',N,S, 'LowerBound',0);

CAPEX = c1_eTES*eTES + c1_pTES*pTES ;

OPEX_norm = 0;

for s = 1:S
    OPEX_norm = OPEX_norm + 365*20*prob_s(s)*sum(QDump_cost(:,s).*QDump(:,s)
+QPeak_cost(:,s).*QPeak(:,s)); % Factor Updated for 1 year Design Life
%     OPEX_norm = OPEX_norm + 52*1*prob_s(s)*sum(QDump_cost(:,s).*QDump(:,s) +
QPeak_cost(:,s).*QPeak(:,s)); % Factor Updated for 1 year Design Life

```

```

end

TESprob.Objective = CAPEX + OPEX_norm;

% Include Constraints
TESprob.Constraints.TESin_min_cons = QSupply(:, :) - QDump(:, :) >= 0 ;
TESprob.Constraints.TESout_min_cons = QDemand(:, :) - QPeak(:, :) >= 0 ;
TESprob.Constraints.TESin_max_cons = QSupply(:, :) - QDump(:, :) <= pTES ;
TESprob.Constraints.TESout_max_cons = QDemand(:, :) - QPeak(:, :) <= pTES ;

TESprob.Constraints.ETES_max_cons = ETES <= eTES*ones(N,S) ;

% ETES Evolution Constraints
cons_ETESevol = optimconstr(N,S);

cons_ETESevol(1,:) = ETES(1,:) - ETES0 == QSupply(1,:) - QDump(1,:) -
(QDemand(1,:) - QPeak(1,:)) - beta*ETES(1,:);
for k = 2:N
    cons_ETESevol(k,:) = ETES(k,:) - ETES(k-1,:) == QSupply(k,:) - QDump(k,:) -
(QDemand(k,:) - QPeak(k,:)) - beta*ETES(k,:);
end

TESprob.Constraints.ETESevol_cons = cons_ETESevol;

t = toc;
run_time{2,1} = ['Define Problem_', num2str(t)];

%% Solving Large LP

% Converting to Matrix form
tic
TESproblem = prob2struct(TESprob);
t = toc;
run_time{4,1} = ['Large LP Generate Matrix_', num2str(t)];

% Solving using CPLEX
tic
options = cplexoptimset;

opt_sol = cplexlp(TESproblem.f, TESproblem.Aineq, TESproblem.bineq, TESproblem.Aeq,
TESproblem.beq, TESproblem.lb, TESproblem.ub);
t = toc;
run_time{5,1} = ['Large LP Solve_', num2str(t)];

% Variables in Order :- ETES, QDump, QPeak, eTES, pTES
% ideTES = varindex(TESprob, 'eTES')
% idpTES = varindex(TESprob, 'pTES')
ideTES = size(TESproblem.ub, 1) - 1;
idpTES = size(TESproblem.ub, 1);

```

```

for s = 1:S
opt_ETES(:,s) = opt_sol( N*(s-1) + 1 : N*s);
opt_QDump(:,s) = opt_sol( N*S+ N*(s-1) + 1 : N*S + N*s);
opt_QPeak(:,s) = opt_sol( 2*N*S+ N*(s-1) + 1 : 2*N*S + N*s);
end

% run_time
opt_x = [opt_sol(idetES); opt_sol(idpTES)]
opt_vol_area = opt_x.*[1000*3600/62760; 1000000/(18.2*850)] % Converting eTES and
pTES to volume and area

%% Plotting

plot_scenario_start = 1;

plot_scenario_end = 1;

for s = plot_scenario_start:plot_scenario_end

fig1 = figure; %%Supply, Demand and Prices

subplot(2,1,1);
plot(Days_plot(:,1), QSupply(:,s), 'r');
hold on;
plot(Days_plot(:,1), QDemand(:,s), 'b');
legend('QSupply', 'QDemand'); xlabel('Days'); ylabel('Energy in MW');
title("Scenario " + s);

subplot(2,1,2);
plot(Days_plot(:,1), QPeak_cost(:,s), 'r');
legend('QPeak_cost'); xlabel('Days'); ylabel('QPeak_cost in USD/MWh');

fig2 = figure;

subplot(2,1,1);
plot(Days_plot(:,1), QSupply(:,s), 'r');
hold on;
plot(Days_plot(:,1), QSupply(:,s) - opt_QDump(:,s), 'b');
legend('QSupply', 'Qtes,in'); xlabel('Days'); ylabel('Energy in MW');
title("Scenario " + s);

subplot(2,1,2);
plot(Days_plot(:,1), QDemand(:,s), 'b');
hold on;

```

```

plot(Days_plot(:,1), QDemand(:,s) - opt_QPeak(:,s), 'r');
legend('QDemand', 'Qtes,out'); xlabel('Days'); ylabel('Energy in MW');

fig3 = figure;

subplot(2,1,1);
plot(Days_plot(:,1), opt_ETES(:,s), 'c');
legend('Etes'); xlabel('Time in Hours'); ylabel('Etes in MWh');
ylim([0,15]);
title("Etes Scenario " + s);

subplot(2,1,2);
plot(Days_plot(:,1), QSupply(:,s) - opt_QDump(:,s), 'r');
hold on
plot(Days_plot(:,1), QDemand(:,s) - opt_QPeak(:,s), 'b');
legend('Qtes,in', 'Qtes,out'); xlabel('Time in Hours'); ylabel('Energy in MW');

iptwindowalign(fig1, 'right', fig2, 'left');
iptwindowalign(fig1, 'bottom', fig2, 'top');
iptwindowalign(fig1, 'left', fig3, 'right');
end

if eTES_max == 0
    c0_eTES = 0;
end

opt_CAPEX = TESproblem.f(end-1:end)*opt_sol(end-1:end) + c0_eTES + c0_pTES
opt_OPEX = TESproblem.f(1:end-2)*opt_sol(1:end-2)

```