Chemical Kinetics and Thermal Hydraulics of Lead Bismuth Flow Loops

Kanthi Kiran Dasika
University of Nevada, Las Vegas

Follow this and additional works at: https://digitalscholarship.unlv.edu/thesesdissertations
Part of the Mechanical Engineering Commons, Mechanics of Materials Commons, and the Nuclear Engineering Commons

Repository Citation
https://digitalscholarship.unlv.edu/thesesdissertations/1500

This Thesis is brought to you for free and open access by Digital Scholarship@UNLV. It has been accepted for inclusion in UNLV Theses, Dissertations, Professional Papers, and Capstones by an authorized administrator of Digital Scholarship@UNLV. For more information, please contact digitalscholarship@unlv.edu.
CHEMICAL KINETICS AND THERMAL HYDRAULICS OF LEAD BISMUTH FLOW LOOPS

by

Kanthish Dasika

Bachelor of Science in Mechanical Engineering
College of Engineering, Andhra University, Visakhapatnam, India
May 2000

A thesis submitted in partial fulfillment of the requirements for the

Master of Science Degree in Mechanical Engineering
Department of Mechanical Engineering
Howard R. Hughes College of Engineering

Graduate College
University of Nevada, Las Vegas
December 2003
ABSTRACT

Chemical Kinetics and Thermal Hydraulics of Lead bismuth Flow Loops

by

Kanthi Kiran Dasika

Dr. Samir Moujaes & Dr. Yitung Chen, Examination Committee Chairs
Professors of Mechanical Engineering
University of Nevada, Las Vegas

The objective of the thesis is to study the effect of chemical kinetics and thermal hydraulics of Lead Bismuth Eutectic (LBE) flow in the Materials Test Loop (MTL). The Materials Test Loop, also known as the Delta Loop, was built in Los Alamos National Laboratories (LANL) to obtain the experimental data for corrosion estimation and analysis. It is a well-known fact that corrosion plays an important role in the design of nuclear thermal hydraulic systems. Since the MTL is a multi-section closed system that differs in diameter from one part to another, an intensive study on the overall and regional corrosion distribution is necessary and valuable. In previous studies, experimental data on this research area is very limited and far from accurate and complete.

Flow simulations using a commercial Computational Fluid Dynamics code, analysis of the flow dynamics and estimation of corrosion in the MTL due to the LBE flow, by assuming simplified geometries for the MTL, are the topics of discussion. For the flow analysis and corrosion estimation, three simplified geometries of the MTL have been assumed, results from one assumption leading to the other. Wall concentrations obtained
from previous analytical studies have been used to impose the boundary conditions on the model.

Results from flow simulation and theoretical analyses have been compared which seem to be in good agreement. The improvement in this work is the prediction of the corrosion flux at elbows due to the multidirectional nature of the flow. The results are beneficial for the future design of the thermal hydraulic loop to minimize corrosion at critical points.
TABLE OF CONTENTS

ABSTRACT........................................................................................................................................ iii

LIST OF FIGURES ..................................................................................................................... vii

ACKNOWLEDGMENTS ........................................................................................................... x

CHAPTER 1  INTRODUCTION AND BACKGROUND ......................................................... 1

1.1. Nuclear Waste Treatment ............................................................................................ 1
1.2. Lead Bismuth Eutectic................................................................................................. 2
1.3. Active Oxygen Control............................................................................................... 4
1.4. Materials Test Loop (MTL)....................................................................................... 5
1.5. Kinetics of Chemical Corrosion............................................................................... 7

CHAPTER 2  NUMERICAL TECHNIQUES AND MODEL DESCRIPTION ..................... 14

2.1. Numerical Simulation Technique .......................................................................... 14
2.2. Model Description ................................................................................................. 24
   2.2.1. Straight Pipe Model ........................................................................................ 27
   2.2.2. Toroidal Loop Model...................................................................................... 29
   2.2.3. Rectangular Loop Model .............................................................................. 32

CHAPTER 3  RESULTS AND DISCUSSION .................................................................. 34

3.1. Straight Pipe Model ............................................................................................... 34
   3.1.1. Benchmark Study............................................................................................ 35
      3.1.1.1. Laminar Flow........................................................................................ 35
      3.1.1.2. Turbulent Flow....................................................................................... 38
   3.1.2. Parametric Study............................................................................................. 45
      3.1.2.1. Reynolds Number.................................................................................. 46
      3.1.2.2. Schmidt Number.................................................................................... 47
      3.1.2.3. Initial Oxygen Concentration................................................................. 49
      3.1.2.4 Temperature Gradient along the Loop Length....................................... 51
   3.2. Toroidal Loop Model............................................................................................. 54
   3.3. Rectangular Loop Model ..................................................................................... 58
3.3.1. Benchmark Study.......................................................................................................................... 58
  3.3.1.1 Laminar Flow.............................................................................................................................. 58
  3.3.1.2 Turbulent Flow.......................................................................................................................... 70
3.3.2. Parametric Study............................................................................................................................. 82
  3.3.2.1 Reynolds Number ...................................................................................................................... 82
  3.3.2.2 Schmidt Number ...................................................................................................................... 84
  3.3.2.3 Initial Oxygen Concentration.................................................................................................. 86
  3.3.2.4 Temperature Variation across the Loop Length ...................................................................... 87

CHAPTER 4 CONCLUSIONS ....................................................................................................................... 90

BIBLIOGRAPHY ........................................................................................................................................ 91

VITA ......................................................................................................................................................... 93
LIST OF FIGURES

Figure 1  Materials Test Loop ........................................................................................... 6
Figure 2  Imposed wall temperature and concentration for the MTL ............................. 26
Figure 3  Straight pipe model .......................................................................................... 28
Figure 4  Toroidal Loop Model ....................................................................................... 31
Figure 5  Rectangular Loop Model .................................................................................. 33
Figure 6  Velocity profile at the end section of the 5m straight pipe model of the MTL 35
Figure 7  Temperature profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL .................... 36
Figure 8  Concentration profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL .................... 37
Figure 9  Velocity profile at the end section of the 5m straight pipe model of the MTL 38
Figure 10 Temperature profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL .................... 39
Figure 11 Concentration profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL .................... 39
Figure 12 Corrosion/Precipitation Rate for a Turbulent Open Straight Pipe Model Assumption of the Materials Test Loop from Analytical Model............. 40
Figure 13 Corrosion/Precipitation Rate for a Laminar Open Straight Pipe Model Assumption of the Materials Test Loop from Simulation Model.................. 41
Figure 14 Corrosion / Precipitation Rate for a Turbulent Open Straight Pipe Model Assumption of the Materials Test Loop from Simulation Model.................. 42
Figure 15 Grid Independency Check for a Laminar Straight Pipe Flow......................................... 42
Figure 16 Grid Independency Check for a Turbulent Straight Pipe Flow................................. 44
Figure 17 Parametric study in Reynolds number for a turbulent open straight pipe model ......................................................................................................................... 46
Figure 18 Parametric study in Schmidt number for a laminar open straight pipe model. 48
Figure 19 Parametric study in Schmidt number for a turbulent open straight pipe model 48
Figure 20 Parametric study in the initial oxygen concentration for a laminar open straight pipe model ......................................................................................................................... 50
Figure 21 Parametric study in the initial oxygen concentration for a turbulent open straight pipe model ......................................................................................................................... 51
Figure 22 Parametric study in the temperature gradient across the loop length for a laminar open straight pipe model .......................................................... 52
Figure 23 Parametric study in the temperature gradient across the loop length for a turbulent open straight pipe model .......................................................... 53
Figure 24 Velocity profile due to turbulent flow at the main test section in the closed toroidal loop model ......................................................................................... 55
Figure 25 Temperature profile due to the turbulent flow at the main test section in the closed toroidal loop model ......................................................................................... 55
Figure 26 Concentration profile due to the turbulent flow at the main test section in the closed toroidal loop model................................................................. 56
Figure 27 Corrosion/Precipitation Rate for a Turbulent Closed Straight Loop Model Assumption of the Materials Test Loop......................................................... 56
Figure 28 Corrosion/Precipitation Rate for a Turbulent Closed Toroidal Loop Model Assumption of the Materials Test Loop......................................................... 57
Figure 29 Velocity Profile in the Overall Loop Length for a Laminar Rectangular Loop Model ...................................................................................................... 59
Figure 30 Velocity Profile at an Elbow Section of the Laminar Rectangular Loop Model ........................................................................................................ 60
Figure 31 Temperature Profile in the Overall Loop Length for a Laminar Rectangular Loop Model ........................................................................................ 60
Figure 32 Concentration Profile in the Overall Loop Length for a Laminar Rectangular Loop Model ....................................................................................... 61
Figure 33 Concentration Profile at an elbow section for a Laminar Rectangular Loop Model ................................................................................................. 61
Figure 34 Corrosion/Precipitation rate for a laminar closed rectangular loop model assumption of the Materials Test Loop......................................................... 62
Figure 35 Velocity contour at the first elbow cut away section normal to the flow ...... 64
Figure 36 Concentration profile at the first elbow cut away section normal to the flow . 64
Figure 37 Velocity contour at the second elbow cut away section normal to the flow.... 65
Figure 38 Concentration profile at the second elbow cut away section normal to the flow ................................................................................................. 66
Figure 39 Velocity contour at the third elbow cut away section normal to the flow ...... 66
Figure 40 Concentration profile at the third elbow cut away section normal to the flow 67
Figure 41 Velocity profile on the edges of the elbow section........................................ 68
Figure 42 Rate of corrosion change on the edges of an elbow section ................. 68
Figure 43 Grid Independency Check for a Laminar Rectangular Loop Model............ 69
Figure 44 Velocity profile in the overall loop length for a turbulent rectangular loop Model ........................................................................................................ 70
Figure 45 Velocity profile at an elbow section for a turbulent rectangular loop model.. 71
Figure 46 Temperature profile in the overall loop length for a turbulent rectangular loop Model ........................................................................................................ 71
Figure 47 Temperature profile at an elbow section for a turbulent rectangular loop model ........................................................................................................ 72
Figure 48 Concentration profile in the overall loop length for a turbulent rectangular loop Model ........................................................................................................ 73
Figure 49 Concentration profile at an elbow section for a turbulent rectangular loop model........................................................................................................ 73
Figure 50 Corrosion/Precipitation rate for a turbulent closed rectangular loop model assumption of the Materials Test Loop......................................................... 75
Figure 51 Velocity profile on the edges of the elbow section........................................ 75
Figure 52 Corrosion/Precipitation rate on the edges of the elbow section............... 76
Figure 53 Velocity contour at the first elbow cut away section normal to the flow ...... 77
Figure 54 Concentration profile at the first elbow cut away section normal to the flow . 78
Figure 55 Velocity contour at the second elbow cut away section normal to the flow.... 78
Figure 56 Concentration profile at the second elbow cut away section normal to the flow .......................................................... 79
Figure 57 Velocity contour at the first elbow cut away section normal to the flow ...... 80
Figure 58 Concentration profile at the first elbow cut away section normal to the flow . 80
Figure 59 Grid independency check for a turbulent rectangular loop model............ 81
Figure 60 Parametric Study in Reynolds Number for Turbulent K-ε Flow ............... 83
Figure 61 Parametric study in Schmidt number for laminar rectangular loop model ...... 85
Figure 62 Parametric study in Schmidt number for a turbulent rectangular loop model . 85
Figure 63 Parametric Study in Initial Oxygen Concentration for Laminar Flow.......... 86
Figure 64 Parametric Study in Initial Oxygen Concentration for Turbulent Flow ......... 87
Figure 65 Parametric study of the Temperature variation along the Loop Length for a Laminar Regime.......................................................................................................................... 88
Figure 66 Parametric study of the Temperature variation along the Loop Length for a Turbulent Regime .......................................................................................................................................... 89
ACKNOWLEDGMENTS

I would like to acknowledge help and esteemed guidance of the Project Investigators Dr. Samir Moujaes and Dr. Yitung Chen for providing supervision and assistance with every step of the work.

Support from the industrial contacts Dr. Ning Li and Dr. Jinsuo Zhang is greatly appreciated. I would also like to thank the Department of Energy for funding this project. I would like to extend my sincere gratitude to Dr. Anthony Hechanova, Director, Transmutation Research Program at University of Nevada, Las Vegas.

My sincere acknowledgements to my project mate Mr. Chao Wu, who assisted me in my work all through the way.
CHAPTER 1

INTRODUCTION AND BACKGROUND

1.1. Nuclear Waste Treatment

An Accelerator Transmutation of Waste (ATW) based project to develop a future capability to separate actinides and long lived fission products from spent fuel, to transmute them, and to dispose off the remaining waste in optimal form, was developed at the Los Alamos National Laboratory (LANL). This project has been developed by multi-machine laboratories managed by the U.S. Department of Energy, involving several technologies like, separation technology, accelerator technology and transmutation technology. Transmutation technology has been mainly emphasized in the discussion below.

Transmutation is a nuclear transformation that effectively converts one isotope into another. Nuclear spent fuel, after producing nuclear energy in the form of heat for several years, still contains minor amounts of transuranics (mainly plutonium) and useful potential energy. This is considered as waste in many nations because of the decreased reactivity due to the consumption of $^{235}$U, buildup of fission and activation products, and degradation of mechanical integrity. The process involving the conversion of these transuranic isotopes and long-lived fission products into short-lived isotopes is called transmutation. Exposing these isotopes to neutrons in either a critical nuclear reactor or
an accelerator-driven sub critical nuclear system are the efficient methods for nuclear transmutation.

Two main technologies that come under the transmutation technology are the fuel/blanket and spallation target. While fuel/blanket technology includes the options of molten salt thermal systems, liquid metal fast reactors and gas cooled systems, spallation target includes gas cooled tungsten, integral lead-bismuth target and coolant, and others. Liquid fuel forms prove to be advantageous to the designer. Due to significant advantages of liquid lead-bismuth over sodium, as both a spallation target and as a coolant, it was designated the preferred technology [1].

1.2. Lead Bismuth Eutectic

The usage of Lead Bismuth Eutectic (LBE) for the U.S. DOE Transmutation Research Program (TRP), of which ATW was a part, as a coolant and target material was under consideration in the United States from 1950’s [2, 3]. The main reason leading to the consideration of LBE for this project was its successful usage in Russian submarine nuclear reactors [4]. LBE is an alloy of 43.6% lead, 55.8% bismuth and few other components adding up to less than 0.032% by weight. Different aspects of LBE that attracted scientists over the years are its unique nuclear, thermo-physical and chemical properties. Its high spallation neutron production when bombarded with protons (30 neutrons per 1 GeV proton), low neutron capture and shielding against the gamma rays makes it an attractive nuclear target [5, 6]. It has a very low melting point (~123.5°C) and a high boiling point (1725°C) along with excellent heat transfer properties [4]. From the reactor design point of view using LBE coolant, its small volume change upon
solidification does not damage the structural components due to coolant freezing, and natural circulation capability steers clear of the primary coolant pumps. Its non-reactivity with air and water make it chemically more proven than liquid sodium.

The main drawback, though, in using LBE is its high reactivity with common steels used in nuclear coolant applications, leading to corrosion. Solubility of Ni, Fe, Cr and other major alloying components of steel can reach a few weight percent at moderately high temperatures resulting in corrosion. Additionally, the solubility is a function of temperature. Previous research proved that higher chromium percentage in the steels consequences in higher rate of corrosion. Use of the refractory materials like Mo, W and Ta are totally obdurate to LBE, but the usage of these materials is not pragmatic. Usage of additives like Zr, Ti and Mg or prior coating of the structural materials with nitride or oxide proved to be futile in preventing the steels from corroding [2].

Tests involving the smearing of insoluble coatings like nitrides or alumina resulted in abrasion and cuts causing the chipping of flakes due to the flow and instigated in more severe corrosion. The maintenance of the concentration of inhibitors such as Ti or Zr, and the presence of adequate amount of nitrogen in steels, for forming of protective coating of nitrides, is crucial for long service, as failing to do so results in the contamination of the steel structures. Pre-oxidation of the steel surfaces also proved futile [3].

However, some tests conducted by the Russians revealed that corrosion attack can be minimized by the existence of an oxide layer on the steel surface. Stability of this film is very crucial for the undisturbed running of the nuclear reactor, and is mainly dependent on the oxygen concentration in the coolant. Deviation in the oxygen concentration in the LBE coolant from a narrow range leads to many complications. Low concentration levels
result in a reducing environment that would dissolve the oxide. If the concentration levels are too high, the precipitation of oxide slag could foul the heat transfer surfaces and/or clog the flow channels [6]. The theory behind the maintenance of the levels of oxygen concentration is explained by “Active Oxygen Control” technique, which is discussed in the next section.

1.3. Active Oxygen Control

Major components of steel like Fe, Cr and Ni are highly reactive with LBE. The principle behind the application of active oxygen control technique is the fact that these components of steel are more vigorous towards oxygen than lead and bismuth. If oxygen concentration levels are maintained in the LBE, the iron and chromium present in the steel react with the oxygen and form a protective layer of oxides, and protect the liquid metal from excessive oxidation resulting in less corrosion. This protective film mainly separates the much reactive chromium from the LBE. The longevity of this film is preserved by controlling the oxygen concentration in the LBE. The film mainly slows down the dissolution to a considerable extent, as the diffusion of the alloying components is very small in the oxides. The transfer of the structural material into the liquid metal is also possible through reduction of this oxide layer. But this reduction will reach a local equilibrium resulting in a attaining an equilibrium for the iron concentration, which is mainly dependent on the oxygen concentration in LBE. Thus, controlling the oxygen concentration in a certain range helps keep the Fe concentration several orders of magnitude less than the Fe solubility in LBE. This facilitates the reduction of surface
depletion to an acceptable value for long-standing applications. This briefly describes the oxygen control technique [5].

1.4. Materials Test Loop (MTL)

To perform the thermal hydraulics and material compatibility testing of liquid LBE and steel walls of the nuclear reactor, an experimental setup called the Materials Test Loop (MTL) has been constructed [2]. The MTL was designed by the Los Alamos National Laboratory (LANL) team members in cooperation with Institute of Physics and Power Engineering (IPPE), Obninsk, Russia, and named it as DELTA ((DEvelopment of Lead-Bismuth Target Applications) loop [4]. The MTL is also used to develop candidate materials with oxygen control [7]. The main goals of DELTA loop are:

- Implementation of an oxygen measurement and control system in the LBE flow.
- Investigation of the long-term corrosive effects of LBE on a variety of materials.
- Implementation and investigation of natural convection flow in an LBE system.
- Investigation of the thermal-hydraulic properties of LBE in prototype target designs [8].

The DELTA loop is shown in Figure 1. It is a closed loop consisting of a pump, piping, heat exchangers and tanks. During operation, lead-bismuth is melted in the Melt Tank, transferred by gas pressure into the Sump Tank. A centrifugal pump submerged in the liquid metal in the Sump Tank circulates the fluid through the loop. After leaving the Sump Tank, liquid lead-bismuth travels up to the Recuperator’s shell side where the fluid’s temperature is increased by 100°C.
A magnetic flow meter is placed on the long vertical pipe leading from Recuperator’s shell side to the heated section at the bottom of the loop. Band heaters cover the next five horizontal tubes. There the fluid’s temperature is raised another 50°C.

Figure 1: Materials Test Loop [8]

The fluid leaves the heat exchanger through the bottom outlet, goes down through the vertical pipe, turns and returns to the Sump Tank through the bottom inlet. Several pipes
are built into the loop to allow bypass of the Recuperator, Heat Exchanger or the Sump Tank. The pump used in MTL is a standard centrifugal pump with an 8.5 in impeller. It is driven by a 25 horse power electric motor and is capable of 58 GPM maximum flow in the loop. The recuperator is standard shell and tube heat exchanger where both the hot and cold fluids are liquid lead-bismuth at different temperatures. The heat exchanger consists of several concentric tubes with water as the cooling fluid. Water is separated from the loop fluid by an annulus filled with lead-bismuth. All components of the loop are built of standard 316 stainless steel, which is one of the materials to be tested for its interaction with lead-bismuth. MTL also has a test section where coupons of various other materials can be placed for testing in the lead-bismuth flow [4].

1.5. Kinetics of Chemical Corrosion

In the past few years, several different analytical models, describing the kinematics of precipitation and corrosion in LBE flow loops, have been developed. These models included the studies in both the isothermal and non-isothermal loops. One of the main assumptions in most of these models developed is that there are no bends or complicated geometries involved. The flow is assumed to be in a straight pipe with the fluid coming out of the pipe from one run, fed as an inlet for the next run with same outlet conditions. A brief description of the various models, with different parameters developed before, have been presented in this chapter.

As explained in the previous chapter, the Materials Test Loop, as the name indicates, is material testing equipment that has been developed by the Los Alamos National Laboratories team. The geometry of the MTL is very complicated, involving a heater,
recuperator and heat exchanger to set and control temperature variations. LBE is pumped from the melt tank using a centrifugal pump at 350°C. The LBE is then allowed to flow through the recuperator, where it is heated to 450°C, by absorbing the heat from the LBE coming from the test section. It is then passed through the main heating section, where the temperature is raised to 550°C. It then passes through the test section and then enters the recuperator, where it exchanges heat with the liquid coming from the pump resulting in a temperature drop of 100°C. The temperature is further reduced to 350°C, when it passes through a heat exchanger on its way back to the melt tank [5].

The flow dynamics, the temperature variations along the loop length and the LBE reactivity with iron and oxygen result in corrosion of the steel structure. The corrosion of this steel structure usually occurs in two different ways, namely, dissolution and reduction. Without the presence of oxygen coating, the dissolution of iron occurs according to the formula:

$$\text{Fe(S)} \rightarrow \text{Fe(Sol)} \quad (1)$$

The solubility of iron in LBE can be expressed as

$$\log(c) = \log(c_s) = 6.01 - \frac{4380}{T} \quad (2)$$

where T is the absolute temperature.

Let us now consider the case where there is oxygen introduced into the flow. Oxygen in the MTL mostly stays as lead oxide. The lead-oxide reacts with iron on the surface according the reduction formula given below:

$$4\text{Pb} + \text{Fe}_3\text{O}_4(S) \rightarrow 3\text{Fe} + 4\text{PbO(Sol)} \quad (3)$$

The equilibrium concentration of Fe, for the above reaction, can be obtained as,

$$\log(c_{Fe}) = 11.35 - \frac{12844}{T} - \log(c_o) \quad (4)$$
where, $c_{Fe}$ is the concentration of iron and $c_o$ is the concentration of oxygen introduced into the LBE [3].

Balboud-Celerier and Barbier developed an analytical expression for predicting the corrosion rate, which is given by [9]:
\[
q = K*(c_{surf} - c_{bulk}) \tag{5}
\]
where $q$ is the corrosion/precipitation rate, $K$ is the mass transfer coefficient, $c_{surf}$ is the corrosion product concentration at the solid-liquid interface and $c_{bulk}$ is the bulk concentration of the liquid metal flowing in the loop.

Several expressions for calculating the mass transfer coefficient have been developed in the past. The analytical expression developed by Pinczewski and Sideman in 1974 expresses the mass transfer coefficient as shown below [10]:
\[
K_{P-S} = \frac{3}{[2\Gamma (1/3)]} \left( \frac{3}{1740} \right)^{1/3} \nu^{-2/3} D^{2/3} u \left( \frac{\lambda}{2} \right)^{1/2} \tag{6}
\]
where $\Gamma$ is the Gamma function. The friction factor $\lambda$, according to Blasius equation, is given by, $\lambda = 0.079Re^{-0.25}$ where $Re$ is the Reynolds number. Assuming, $\Gamma (1/3) = 2.6789$, equation 6 can be reduced as [11]:
\[
K_{P-S} = 0.0133\nu^{-0.542} D^{0.667} u^{0.875} d^{-0.125} \tag{7}
\]
where, $\nu$ is the kinematic viscosity, $D$ is the mass diffusion coefficient, $u$ is the mean flow velocity and $d$ is the hydraulic diameter for the above expression and the expressions that follow.

Following are the expressions for the mass transfer coefficient for a closed loop circular cross-sectional flow, developed by Berger and Hau [12], Silverman [13], and Harriott and Hamilton [14].
\[
K_{B-H} = 0.0203\nu^{-0.530} D^{0.670} Q^{0.860} d^{-1.860} \tag{8}
\]
\[ K_{\text{Silverman}} = 0.0219 \nu^{-0.579} D^{0.704} Q^{0.875} d^{-1.875} \]  
\[ K_{\text{H-H}} = 0.0133 \nu^{-0.567} D^{0.654} Q^{0.913} d^{-1.875} \]  

There are two more unknowns in equation 5. The first unknown, i.e., \( c_{\text{surf}} \) can be determined by solving the equations 2 and 4 that results in an empirical formula that gives the concentration of iron in terms of temperature and oxygen concentration in the LBE [5]. The resulting empirical formula, given below, has been used for simulating the flow in the MTL and calculating the mass diffusion of iron into the fluid by many different researchers.

\[ c_{\text{Fe}} = c_{\text{surf}} = \min \left( c_o^{4/3} \times 10^{11.35 - (12844/T)}, 10^{6.01 - (4380/T)} \right) \]

The second unknown in equation 5, i.e., bulk concentration, \( c_{\text{bulk}} \), for a steady state is given by,

\[ c_{\text{bulk}} = \frac{\int_{0}^{L} s(x) k(x) c_{\text{surf}}(x) \, dx}{\int_{0}^{L} s(x) k(x) \, dx} \]

where, \( L \) is the loop length, \( s(x) \) is the circumference and \( K(x) \) is the local mass transfer coefficient [11].

Expressions have also been developed for the minimum concentrations of oxygen and iron to sustain the formation of the oxide film on the internal pipe surface [6].

\[ c_{o, \text{min}} = c_o^{s, e} \left( \frac{\Delta G_{\text{film}}(T)}{4RT} \right) \]
\[ c_{Fe, min} = c_{Fe, s} \frac{e^{\frac{3RT}{4}}} {\left( \frac{c_o}{c_s} \right)^3} \]

where \( \Delta G_{film}(T) \) is the free energy variation given by,

\[ \Delta G_{film}(T) = -225.6 - 0.143T \quad (15) \]

Various flow dynamic equations and mass diffusion equations used to develop the kinetic models for the mass diffusion of iron into the LBE are presented below. Also shown below are the final expressions for the corrosion/precipitation rate acquired by scientists for different MTL conditions.

The mass transport equation in its general form can be written as:

\[ \frac{\partial c}{\partial t} + (u \cdot \nabla) c = D \nabla^2 c + q \quad (16) \]

where, \( c \) is the concentration, \( u \) is the velocity of the fluid, \( D \) is the diffusivity and \( q \) is the net production or depletion of mass due to corrosion.

The correlation between the hydraulic laminar sublayer and the thickness of the mass diffusion boundary layer is determined by Schmidt number [15], which is defined as,

\[ Sc = \nu/D \quad (17) \]

The mass transfer boundary layer gets thinner, as the Schmidt number goes higher, and for sufficiently high Schmidt number, the mass transfer boundary is submerged under the hydraulic laminar sublayer.

With the assumptions that the diffusion is dominant in the transverse direction and the convection is dominant in the longitudinal direction, and that the diffusion is confined to
a thin layer near the pipe walls, the corrosion/precipitation rate or the species flux at the wall surface, in the general form, for a steady state flow, is then obtained as [16]:

\[
q = -D \left( \frac{\partial c}{\partial y} \right)_{y=0} \left( \frac{2 \pi \gamma D^2}{3L} \right)^{1/3} \frac{1}{\Gamma \left( \frac{1}{3} \right)} \sum_{n \neq 0} c_n n^{1/3} \exp \left( 2 \pi n i \xi + i \frac{i \pi}{6} \right) + \frac{D}{\delta_D} \left[ c_o - (c_o)^b \right]
\]

where, \( \xi = x/L, \ \eta = (\gamma/dL)^{1/3} y, \) \( x \) and \( y \) are the coordinates in the axial and transverse directions respectively, \( \gamma \) is the shear rate at the wall, \( L \) is the loop length and \( d \) is the diameter of the pipe, \( \delta_D \) is the thickness of the concentration boundary layer, \( c_o \) is the average wall concentration, \( (c_o)^b \) is the average bulk concentration.

Transient flow is not involved in the present study. But it is not incongruous here to mention that expressions have been developed by Zhang and Li in [17], for the corrosion/precipitation rate in the MTL for a transient condition.

Zhang and Li, extended their study further to give expressions for the corrosion/precipitation rate for the following. An isothermal loop, a non-isothermal open straight pipe and a non-isothermal closed loop for steady state have been considered, the expressions of which are given below [16].

For an open isothermal pipe flow, the corrosion flux equation is given as,

\[
q = \frac{D}{\delta_D} \left[ c_o - (c_o)^b \right] = k(c_o - c_{\text{bulk}})
\]

Since the flow is in an open pipe, the concentration of the bulk is almost equal to the inlet concentration, which is usually taken as zero. This applies even for the next equation, which gives an empirical formula for the corrosion/precipitation rate for a non-isothermal open pipe flow.
Finally, the corrosion/precipitation rate for a closed loop case (for an MTL) is given according to the below given formula:

\[
q = \left( \frac{2 \pi D^2}{3L} \right)^3 \frac{1}{\Gamma\left(\frac{1}{3}\right)} \sum_{n} \frac{1}{n^3} \exp\left(2\pi ni\xi + i\frac{\pi}{6}\right) + K\left[c_o - \left(c_o\right)^b\right]
\]

(20)

Graphs depicting the corrosion or precipitation rate for a straight pipe and the MTL, using the above expressions have been expounded, the details of which will be discussed in chapter 3.
CHAPTER 2

NUMERICAL TECHNIQUES AND MODEL DESCRIPTION

This chapter provides information on the working theory behind the simulation package used to model the LBE flow in the MTL and the various models considered for simulating the MTL. The chapter is split into two subchapters. The first part provides a detailed description of the operational concept behind the simulation package used for the present study. The second subchapter presents the details of different models that were used for the research purposes.

2.1. Numerical Simulation Technique

The purpose of this study, as explained before, is to simulate the LBE flow in the MTL and to estimate the corrosion of steel pipes due to the reactivity of LBE with iron and oxygen. The Computational Fluid Dynamics (CFD) tool used for this study is called STAR-CD, developed by the Computational Dynamics Ltd. The system comprises the main analysis code STAR (Simulation of Turbulence in Attributed Regions), and the pre-processor and post-processor code, PROSTAR. STAR-CD is a powerful CFD tool for thermo-fluids analysis and has been designed for use in a Computer Aided Engineering environment. It is a finite volume code, developed for the calculation of fluid flow, heat and mass transfer and chemical reaction in industrial and environmental applications. Its many attributes include:
- A self-contained, fully-integrated and user-friendly program suite comprising pre-processing, analysis and post-processing facilities
- A general geometry-modeling capability that renders the code applicable to the complex shapes often encountered in industrial applications
- Extensive facilities for automatic meshing of complex geometries, either through built-in tools or through interfaces to external mesh generators such as SAMM™ and ICEM CFD Tetra™
- Built-in models of an extensive and continually expanding range of flow phenomena, including transients, compressibility, turbulence, heat transfer, mass transfer, chemical reaction and multi-phase flow
- Fast and robust computer solution techniques that enhance reliability and reduce computing overheads
- Easy-to-use facilities for setting up and running very large CFD models using state-of-the-art parallel computing techniques
- Built-in links with popular proprietary CAD/CAE systems, including PATRAN™, IDEAS™ and ANSYS™

STAR, written in FORTRAN 77 and C, operates by solving the governing differential equations of flow physics by numerical means on a computational mesh, while PROSTAR is an interactive, command-driven, combined pre-processor and post-processor whose main functions include geometry modeling and mesh generation, problem specification, results manipulation and display, file control, and links to external CAD/CAE systems. The governing equations used by STAR-CD are given below:
The mass and momentum conservation equations solved by STAR-CD for general incompressible fluid flows and a moving coordinate frame (‘Navier-Stokes’ equations) are, in Cartesian tensor notation:

\[
\frac{1}{\sqrt{g}} \frac{\partial (\sqrt{g} \rho)}{\partial t} + \frac{\partial (\rho \tilde{u}_j)}{\partial x_j} = s_m
\]  \hspace{1cm} (22)

\[
\frac{1}{\sqrt{g}} \frac{\partial (\sqrt{g} \rho u_i)}{\partial t} + \frac{\partial (\rho \tilde{u}_j u_i - \tau_{ij})}{\partial x_j} = -\frac{\partial p}{\partial x_i} + s_i
\]  \hspace{1cm} (23)

where \( t \): time

\( x_i \): Cartesian coordinate \((i=1, 2, 3)\)

\( u_i \): absolute fluid velocity component in direction \( x_i \)

\( \tilde{u}_j \): \( u_j - u_{cj} \), relative velocity between fluid and local (moving)coordinate frame that moves with velocity \( u_{cj} \)

\( p \): piezometric pressure= \( p_s - \rho_0 g_m x_m \), where \( p_s \) is static pressure, \( \rho_0 \) is reference density, the \( g_m \) are gravitational field components and the \( x_m \) are coordinates from a datum, where \( \rho_0 \) is defined

\( \rho \): density

\( \tau_{ij} \): stress tensor components

\( s_m \): mass source

\( s_i \): momentum source components

\( \sqrt{g} \): determinant of metric tensor

and repeated subscripts denote summation.

The specialization of the above equations to a particular class of flow involves:
• Application of ensemble or time averaging if the flow is turbulent

• Specification of a constitutive relation connecting the components of the stress tensor $\tau_{ij}$ to the velocity gradients

• Specifications of the ‘source’, $s_i$, which represents the sum of the body and other external forces, if present.

In case of laminar flows, STAR-CD is applicable to Newtonian fluids that obey the following constitutive relation:

$$\tau_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$  \hspace{1cm} (24)

where $\mu$ is the molecular dynamic fluid viscosity and $\delta_{ij}$, ‘Kronecker delta’, is unity when $i=j$ and zero otherwise. $s_{ij}$, the rate of strain tensor, is given by:

$$s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$  \hspace{1cm} (25)

For turbulent flows, $u_i$, $p$ and other dependent variables, including $\tau_{ij}$, assume their ensemble averaged values (equivalent to time averages for steady-state situations) giving, for equation 28:

$$\tau_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} - \overline{\rho u_i u_j}$$  \hspace{1cm} (26)

where the $u'$ are fluctuations about the ensemble average velocity and the over bar denotes the ensemble averaging process. The rightmost term in the above equation represents the additional Reynolds stresses due to turbulent motion. These are linked to the mean velocity field via the turbulence models.
Heat transfer in STAR-CD is implemented through the following general form of the enthalpy conservation equation for a fluid mixture:

\[
\frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} \rho h) + \frac{\partial}{\partial x_j} (\rho \bar{u}_j h - F_{h,j}) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} p) + \bar{u}_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + s_h
\] (27)

Here, \( h \) is the static enthalpy, defined by:

\[
h \equiv \bar{c}_p T - c^0_p T_0 + \Sigma m_m H_m
\] (28)

and

- \( m_m \): mass fraction of mixture constituent \( m \)
- \( H_m \): heat of formation of constituent \( m \)
- \( \Sigma \): summation over all mixture constituents
- \( \bar{c}_p \): mean constant pressure specific heat at temperature \( T \)
- \( c^0_p \): reference specific heat at temperature \( T_0 \)
- \( s_h \): energy source
- \( h_t \): thermal enthalpy

It should be noted that the static enthalpy \( h \) is defined as the sum of the thermal and chemical components, the latter being included to cater for the chemically reacting flows.

For a constant-density approximation to an ideal gas, e.g. air at standard temperature and pressure, the enthalpy of the gas is transported with all pressure dependent terms ignored, as these are negligible.

For solids and constant density fluids, such as liquids, STAR-CD solves the transport equation for the specific internal energy, \( e \), where:

\[
e \equiv \bar{c} T - c^0 T_0 + \Sigma m_m H_m
\] (29)
where $\bar{c}$ is the mean constant-volume specific heat. This equation is similar in form to equation 31, but does not contain the pressure-related terms. The form of equation 31 appropriate to particular classes of flow is specified via the $F_h$ and $s_h$, as outlined below.

The governing equation for thermal enthalpy is given by:

$$
\frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} \rho h_t) + \frac{\partial}{\partial x_j} (\rho \ddot{u}_j h_t - F_{h,j}) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} p) + \ddot{u}_j \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_j} + s_h - \sum_m m_m H_m s_{c,m}
$$

Here, $h_t$ is the thermal enthalpy, defined by

$$
h_t = \bar{c}_p T - c_p T_0
$$

and $F_{h,j}$: diffusional thermal energy flux in direction $x_j$

$s_{c,m}$: rate of production or consumption of species $m$ due to chemical reaction

A governing equation for total chemico-thermal enthalpy ($H$) may be formed by summing an equation for mechanical energy conservation and static enthalpy equation:

$$
\frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} \rho H) + \frac{\partial}{\partial x_j} (\rho \ddot{u}_j H - u_i \ddot{u}_i) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} p) - \frac{\partial}{\partial x_j} (u_{c,j} p) + s_{u_i} + s_h
$$

where,

$$
H = \frac{1}{2} u_{i,u_i} + h
$$

A governing equation for total thermal enthalpy may be formed in a similar fashion by combining a mechanical energy conservation equation and equation 34.

STAR-CD assumes that the molecular diffusion fluxes of heat and mass obey Fourier’s and Fick’s laws, respectively. Accordingly, for a laminar flow,

$$
F_{h,j} = k \frac{\partial T}{\partial x_j} + \sum_m h_m \rho D_m \frac{\partial m_m}{\partial x_j}
$$

Alternatively,
\begin{align*}
F_{h,j} &= k \frac{\partial T}{\partial x_j} + \sum_m h_{t,m} \rho D_m \frac{\partial m_m}{\partial x_j} \\
\text{(35)}
\end{align*}

where \( k \) is the thermal conductivity, \( D_m \) is the molecular diffusivity of constituent \( m \), and \( h_m, h_{t,m} \) are its static enthalpy and thermal enthalpy, respectively.

For a turbulent flow, heat and mass molecular diffusion fluxes are given as:

\begin{align*}
F_{h,j} &= k \frac{\partial T}{\partial x_j} - \rho \overline{u_j h'} + \sum_m h_m \rho D_m \frac{\partial m_m}{\partial x_j} \\
\text{(36)}
\end{align*}

Alternatively,

\begin{align*}
F_{h,j} &= k \frac{\partial T}{\partial x_j} - \rho \overline{u_j h'} + \sum_m h_{t,m} \rho D_m \frac{\partial m_m}{\partial x_j} \\
\text{(37)}
\end{align*}

where the middle term containing the static enthalpy or thermal enthalpy fluctuations \( h' \) or \( h_{t}' \) represents the turbulent diffusional flux of energy.

Each constituent \( m \) of a fluid mixture, whose local concentration is expressed as a mass fraction \( m_m \), is assumed to be governed by a species conservation equation of the form:

\begin{align*}
\frac{1}{\sqrt{g}} \frac{\partial (\sqrt{g} \rho m_m)}{\partial t} + \frac{\partial (\rho \overline{u_j m_m} - F_{m,j})}{\partial x_j} = s_m \\
\text{(38)}
\end{align*}

where \( F_{m,j} \): diffusional flux component

\( s_m \): rate of production or consumption due to chemical reaction

By analogy with the energy equation, the diffusional flux relation for a laminar flow is

\begin{align*}
F_{m,j} &= \rho D_m \frac{\partial m_m}{\partial x_j} \\
\text{(39)}
\end{align*}

where \( D_m \) is the molecular diffusivity of component \( m \).

The time averaged diffusional flux relation for a turbulent flow is given by:
\[ F_{m,j} \equiv \rho D_m \frac{\partial m_m}{\partial x_j} = \bar{\rho u_j} \bar{m_m} \]  

(40)

where the rightmost term, containing the concentration fluctuation \( m_m \), represents the turbulent mass flux.

In some circumstances, it is not necessary to solve a differential conservation equation for every component of a mixture, due to the existence of algebraic relations between the species mass fractions. An example is the requirement of \( \sum m_m = 1 \)

STAR-CD allows such relations to be exploited, when desired.

All forms of the \( k-\varepsilon \) and \( k-l \) linear models currently contained in STAR-CD assume that the turbulent Reynolds stresses and scalar fluxes are linked to ensemble averaged flow properties in an analogous fashion to their laminar flow counterparts, thus:

\[- \bar{\rho u_i u_j} = 2 \mu_i s_{ij} - \frac{2}{3} (\mu_i \frac{\partial u_i}{\partial x_i} + \rho k) \delta_{ij} \]  

(41)

\[- \bar{\rho u_j h} = \frac{\mu_i}{\sigma_{h,i}} \frac{\partial h}{\partial x_j} \]  

(42)

\[- \bar{\rho u_j m_m} = \frac{\mu_i}{\sigma_{m,i}} \frac{\partial m_m}{\partial x_j} \]  

(43)

where,

\[ k = \frac{\bar{u_i u_i}}{t} \]  

(44)

is the turbulent kinetic energy. The quantity \( \mu_i \) is the turbulent viscosity, \( \sigma_{h,i} \) and \( \sigma_{m,i} \) are the turbulent Prandtl and Schmidt numbers, respectively. The above equations effectively define these quantities. The turbulent viscosity is linked to \( k \) and \( \varepsilon \) via:

\[ \mu_i = f_{\mu} \frac{C_\mu \rho k^2}{\varepsilon} \]  

(45)
or to $k$ and $l$ via:

$$
\mu_t = f_{\mu} C_{\mu}^{1/4} \rho k^{1/2} l
$$

where $C_{\mu}$ is an empirical coefficient, usually taken as a constant, $f_{\mu}$ is another coefficient, to be defined later on. The turbulent Prandtl and Schmidt numbers are also empirical qualities that are usually assigned constant and equal values. An expression relating $k$, $\varepsilon$ and $l$ can be obtained by equating equations 49 and 50. Thus,

$$
l = C_{\mu}^{3/4} \frac{k^{3/2}}{\varepsilon}
$$

The particular high Reynolds number form of $k$-$\varepsilon$ model used in STAR-CD is ‘appropriate’, subject to the caveats given earlier, to fully turbulent, incompressible or compressible flows. It also allows to some extent for buoyancy effects. The transport equations are as follows. Turbulence energy is given by:

$$
\frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} \rho k) + \frac{\partial}{\partial x_j} (\rho \mathbf{\bar{u}}_j k - \frac{\mu_{\text{eff}}}{\sigma_k} \frac{\partial k}{\partial x_j}) = \mu_t (P + P_b) - \rho \varepsilon \frac{2}{3} \left( \frac{\partial u_i}{\partial x_i} + \rho k \right) \frac{\partial u_i}{\partial x_i} + P_{NL}
$$

where

$$
\mu_{\text{eff}} = \mu + \mu_t
$$

$$
P_b \equiv 2 s_{ij} \frac{\partial u_i}{\partial x_j}
$$

$$
P_{NL} = (\mathbf{\bar{u}}_i u_j - 2 s_{ij}) \frac{\partial u_i}{\partial x_j}
$$

$P_{NL} = 0$ for linear models and $\sigma_k$ is an empirical coefficient. The first term on the right-hand side of equation 52 represents turbulent generation by shear and normal stresses and
buoyancy forces, the second viscous dissipation, and the third amplification or attenuation due to compressibility effects. The last term accounts for the non-linear contributions.

The turbulence dissipation rate is given by:

\[
\frac{1}{\sqrt{g}} \rho \frac{\partial}{\partial t} (\sqrt{g} \rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \vec{u}_j \varepsilon - \frac{\mu_{eff}}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j}) = C_{el} \frac{\varepsilon}{k} \left[ \mu_i (P + P_{el} P_{el}) - \frac{2}{3} (\mu_i \frac{\partial u_i}{\partial x_i} + \mu_k) \frac{\partial u_i}{\partial x_i} \right] - C_{e2} \rho \frac{\varepsilon^2}{k} + C_{e4} \rho \frac{\partial u_i}{\partial x_j} + C_{el} \frac{\varepsilon}{k} P_{NL} \tag{53}
\]

The right-hand side terms represent analogous effects to those described above for the \( k \) equation. The turbulent viscosity \( \mu_t \), appearing in the above equation, is obtained via equation 49, with \( f_\mu \) set to unity.

The mixing length model calculates the turbulent viscosity without employing any transport equations, by extending Prandtl’s Mixing Length hypothesis to three-dimensional flows. The model is consistent with the local equilibrium between the turbulent kinetic energy generation and dissipation. The turbulent viscosity is given by:

\[
\mu_t = \rho l_m^2 \left\{ \frac{\partial u_i}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right\}^{1/2} \tag{54}
\]

The mixing length \( l_m \) is given by Van Driest, as:

\[
l_m = ky (1 - e^{-D}) \tag{55}
\]

where

\[
D = \frac{y u_t}{26 \nu} = \frac{y^+}{26} \tag{56}
\]

and

\[
y^+ = \frac{u_t y}{\nu}, \quad u_t = \left( \frac{\tau_w}{\rho} \right)^{1/2}, \quad \tau_w = \left( \mu + \mu_t \right) \frac{du}{dy} \tag{57}
\]
where $y$ is the normal distance from the wall. Equation 58 is valid everywhere between

the wall and a (switching) point, located with in the range $y^+ \approx 60 - 100$, where the

normal $k$-$\epsilon$ transport equations apply. The switching criterion employed is that the

turbulent viscosity given by equation 58 and the one calculated from

$$\mu_t = C_\mu\rho \frac{k^2}{\epsilon}$$ (58)

should be the same to within a specified tolerance. The $k$ and $\epsilon$ values are available from

the solution of turbulence transport equations [18].

2.2. Model Description

This sub-chapter presents the various models that have been created and used for

fluid flow simulation and corrosion estimation in the Materials Test Loop. The overall

study is mainly divided into two parts. The first part is the benchmark study, which

basically talks about comparing the simulation results with the analytical results and

benchmarking the CFD package. The benchmark study also verifies the dependency of

the grid distribution with the outcome of the results i.e., to check that the results are grid

independent. The second part is the parametric study, which details on the results from

the different parametric studies that have been carried out. Primarily, three different

models have been considered to replicate the MTL that have been named as

1. Straight Pipe Model

2. Toroidal Loop Model

3. Rectangular Loop Model
Before going into the details of describing each model, an outline of the different assumptions made needs to be stated. The assumptions specified here are for all the models used for benchmark and parametric study, unless specified.

For all the models that have been considered, the length of the MTL is assumed to be 5m. This is primarily because of the difficulties in running the large length to diameter ratio models using STAR-CD. The 5 m loop length assumption seems to be reasonable, due to the fact that the velocities have been adjusted to be similar to the runs in the original loop for the benchmark study. The overall diameter of the loop is assumed to be uniform and has been taken as 1 inch or 0.025 m. The wall temperatures are assumed to be varying from 623°K to 823°K and the imposed wall concentration is a function of temperature, given by equation 11.

\[ c_{Fe} = c_{surf} = \min \left( c_0^{4/3} \times 10^{11.35 - (12844/T)}, 10^{5.01 - (4380/T)} \right) \] (11)

It is assumed that the flow is incompressible, and that the variation of physical properties of the LBE with the variation of temperature in the given range of 623°K to 823°K is negligible. The table below elaborates on the properties of LBE used for the analysis.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Density ((\rho \ \text{kg/m}^3))</th>
<th>Molecular Viscosity ((\mu \ \text{N/ m}^2))</th>
<th>Specific Heat (C J/KgK)</th>
<th>Thermal Conductivity (K W/mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.018E+04</td>
<td>1.018E-03</td>
<td>1.465E+02</td>
<td>1.419E+01</td>
</tr>
</tbody>
</table>

Table 1: Properties of Lead Bismuth Eutectic
The diffusivity of the iron into the LBE is taken to be 1.0E-08 m²/s for the benchmark study and for most of the cases of the parametric study. The Schmidt number, as explained before is a function of the diffusivity and molecular viscosity, which comes out to be 10 for the case when diffusivity is 1.0E-08 m²/s. The Schmidt number is calculated according to equation 17.

Figure 2: Imposed wall temperature and concentration for the MTL

Figure 2 shows the imposed wall temperature and concentration profiles along the loop length used for the benchmark study and few cases of the parametric study. As can be seen from the figure, the wall temperature varies linearly in the recuperator, heater and heat exchanger zones. The loop length in the figure has been non-dimensionalized. The
units of the wall temperature and wall concentration are in degrees Kelvin and parts per million (ppm) respectively.

Also, for the straight pipe and toroidal loop models, the simulations are carried out in 2D, where as for the rectangular loop model, the simulations are carried out in 3D due to the complexity of the geometry. For the straight pipe and rectangular loop models, a series of parametric studies have been worked out and the simulations included modeling in both laminar and turbulent regimes. Where as, for the toroidal loop model, the simulations did not include the parametric study, nor did they have the studies in the laminar regime, the reasons of which will be detailed in the subsequent discussion. The following subheadings discuss each of the above-mentioned models in detail.

2.2.1. Straight Pipe Model

For this model, the MTL is considered as a straight pipe with a single inlet and single outlet. The model has been assumed as an open pipe where the flow coming out from the outlet will not be fed again into the pipe as inlet for simulating the loop. This axi-symmetric simulation model has a uniform radius of 0.025m and a length of 5m and the LBE enters the pipe with an initial temperature of 623K and an initial concentration of 0ppm, and as specified before, the model has been analyzed as a 2D model. Studies include the flow modeling in both the laminar and turbulent regimes for the benchmark and parametric studies.

Figure 3 shows the skeleton of the straight pipe model considered for the flow analysis. The picture has been zoomed into the inlet region for a clear view of the prototype. As can be seen from the figure, the region near the wall has been refined to a
fair degree. The refinement is necessary to capture the mass diffusion of the species from the wall into the fluid, as the diffusion is very prominent in near the wall region than in the bulk of the fluid.

Figure 3: Straight pipe model

For performing the benchmark study for this model, the simulation has been run with the above-specified assumptions. The benchmark study has been performed in both laminar and turbulent regimes. Care has been taken that the boundary conditions match exactly with the conditions in the DELTA loop and the analytical calculations. For the laminar flow, the fluid is allowed to flow from the inlet at a uniform velocity of 0.004 m/s, and for the turbulent flow, the imposed inlet velocity is 0.4 m/s, which results in the Reynolds numbers of 2000 and 200000 respectively. The wall temperature and concentrations have been set according to figure 2.
To make sure that the results from the runs are not grid dependent, three different mesh structures were created and the results of all the three mesh configurations were compared. The different mesh sizes, in the ‘r’ and ‘z’ directions, taken for the checking the grid independency are,

1. 40 X 2000  
2. 50 X 2000  
3. 60 X 2000

The results from all the three runs have then been compared with the analytical results and then benchmarked. Since the results proved to be grid independent, the model with the minimum number of cells among the three has been chosen for carrying out the parametric study.

A series of parametric studies have been carried out with the chosen model. The parametric studies included runs with different Schmidt numbers, inlet oxygen concentrations, and overall temperature distributions for the laminar regime and turbulent regime. The turbulent regime parametric studies also included the Reynolds number studies. The details of these parametric studies are elaborated in the next chapter.

2.2.2. Toroidal Loop Model

The straight pipe model described above cannot be considered as a replica of the MTL, the primary reason being that the above model is an open pipe, where as the MTL is a closed loop. Though the straight pipe model can predicts the regions of maximal corrosion and precipitation accurately, the actual values are different from the values obtained from the runs, due to the absence of the closed loop condition. The studies for
the straight pipe model have basically been carried out to compare the results with the analytical models and to check the capabilities of the CFD code.

The analytical models that have been developed before, assumed the MTL as a straight loop. The loop situation is simulated by feeding the outlet data from one run as an inlet data for the subsequent run. Attempts were made to carry out the simulations in the same way. But due to some technical difficulties, the runs could not be performed. The main difficulty in creating a straight loop model in STAR-CD is that the inlet position for a run should be exactly at the same geometrical position as the outlet position of the previous run, to feed the data from the outlet as an inlet for the successive run. As can be envisaged, this results in creation of a large number of geometric models for performing a single converged run. This ruled out the creation of a closed straight loop model.

The next closest assumption for the straight loop model is a toroidal geometry with a large radius of curvature. This almost replicates the closed straight loop model, as the secondary flows are negligible in donut shaped geometry with a large radius of curvature. Figure 4 shows the toroidal loop geometry considered for modeling the MTL. As indicated before, the geometry is considered as 2D, due to symmetry.

To replicate the pump, a momentum source term has been incorporated in the model. The momentum source, primarily, acts as a source of flow and continuously pumps the fluid in the model at a uniform velocity at the specified location. In the numerical terms, the fluid is pumped at the specified location, after each iteration. In the process, it transfers all the output results, except the velocity, from one iteration, as input for the
next iteration. Hence, the momentum is not conserved in this process. But this could be neglected, as the elements of primary concern are the temperature and concentration.

![Figure 4: Toroidal Loop Model](image)

Boundary conditions, similar to the straight pipe model, have been applied for this model. One of the main difficulties faced, though, by using the toroidal loop model is a linearly variant temperature profile could not be imposed on the walls. For this reason, the regions, where there was a linear increment or decrement of temperature and concentration on the walls, step increment and step decrement of these variables had to be imposed. Due to this, the results from the runs did not come out favorable. Though the maximal corrosion and precipitation regions seemed to be in good agreement with the analytical results, the graphs showed a few peaks and valleys in the areas where step increment/decrement was approximated for linear increment/decrement.
The model has been run only in the turbulent regime with the mesh distribution of 10 X 2 X 1000. The two divisions in the theta direction have been used for the ease in applying the boundary conditions. Grid independency check or the parametric study was not carried out, due to the dearth of accurate results.

2.2.3. Rectangular Loop Model

As explained before, the assumption of the MTL as a toroidal loop did not yield good results due to the step input approximation for wall temperature. The next closest assumption for the MTL is a closed rectangular loop model with a circular cross section. Because of the non-symmetry, and due to the active participation of the secondary flows due to the elbows present in the rectangular loop model, the geometry can no longer be solved as 2D problem. Hence a 3D model, as shown in the figure 5, has been considered for this case. The region near the wall has been greatly refined for the reasons explained before.

The initial and boundary conditions for this model are same as the ones for the straight pipe model, excepting for the momentum source term. Momentum source has been applied to replicate the pump. The wall temperature and boundary conditions were applied according to figure 2. Benchmark and parametric studies have been carried out in both laminar and turbulent regimes. To check the grid independency for the benchmark study, three different mesh structures have been analyzed as has been done in the straight pipe model case. The mesh distribution in the ‘r’, ‘θ’ and ‘z’ directions are as given below:

1. 24 X 10 X 2000
2. 24 X 20 X 2000
3. 24 X 30 X 2000

Figure 5: Rectangular Loop Model

For this case too, the results came out to be grid independent. Hence, a parametric study has been carried out for the model with the minimum cells. The parameters that have been considered were Reynolds number, Schmidt number, initial oxygen concentration, and temperature variation along the loop length for the turbulent flow. The parameters considered for the laminar flow were Schmidt number, initial oxygen concentration and temperature variation along the loop length. The results of the benchmark study and parametric study will be discussed in detail in the succeeding chapter.
CHAPTER 3

RESULTS AND DISCUSSION

This chapter provides a detailed overview of the results of runs from simulations for all the three MTL model assumptions. Results from the benchmark study are initially compared to the analytical results and then the results from the parametric study are elaborated. The discussion also sheds light on the velocity, temperature and concentration profiles and the effect of concentration flux due to the variation of each of the above parameters. The benchmark and parametric studies have been carried out in both laminar and turbulent regimes.

3.1. Straight Pipe Model

As discussed before, the straight pipe model has been checked for benchmark study and parametric study. The benchmark study primarily consists of comparing the simulation results with the analytical results and checking for the grid independency of the results. The parametric study included the study of the flow dependency on the various parameters and the effect of the flow variations on the corrosion/precipitation rate.
3.1.1. Benchmark Study

This section discusses the hydraulic, thermal and mass transfer behavior of the LBE in the straight pipe model assumption of the MTL. The results from the runs are shown in the form of figures in the following discussion. The discussion is followed by the comparison of the analytical results with the simulation results and thus benchmarking the CFD package. The results are then shown to be grid independent. The grid independency check procedure is outlined in detail later in the section. For the current discussion of the velocity, temperature and concentration profiles, it should be mentioned that the mesh configuration of 50 X 2000 (r x z) has been used for both the laminar flow turbulent flow regimes.

3.1.1.1. Laminar Flow

The velocity profile at the end of the 5m-pipe section of the straight pipe model in the laminar regime is shown in figure 6.

Figure 6: Velocity profile at the end section of the 5m straight pipe model of the MTL
The profile shows only the upper half of the parabola due to the considered geometry of the pie section. The pie geometry considered is due to symmetry. The imposed inlet velocity is 0.004 m/s and the imposed wall temperature and boundary concentration have been applied according to figure 2.

The next parameter of interest is the temperature profile. The imposed wall temperature varies all through out the length of the MTL. For the benchmark study, the temperature along the loop length varies from 623ºK – 823ºK. The fluid enters the inlet at 623ºK. Figure 7 shows the variations in the temperature profile of the LBE due to the variations in the imposed wall temperatures. The section shown in the figure corresponds to the end of the test section and the start of the recuperator zone in the MTL. The wall temperature at the test section is 823ºK and decreases from 823ºK to 723ºK in the recuperator zone.

Figure 7: Temperature profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL.
The diffusion of the temperature into the fluid is clearly visualized in the above figure. The low velocities allow the temperature to diffuse fairly prominently in the transverse direction.

Figure 8: Concentration profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL.

Figure 8 shows the concentration profile of the LBE at the same section. As explained in the previous chapters, the wall concentration is a function of the wall temperature given by equation 11. The flow is allowed at an initial concentration of 0.0 ppm and the wall concentration is given by figure 2. The diffusivity of the iron into the LBE is as low as $1 \times 10^{-8} \text{m}^2/\text{s}$, which makes the diffusion very slow. Due to this, it can be seen that the concentration of the LBE remains at the initial inlet concentration of 0.0 ppm in the bulk of the flow.
3.1.1.2. Turbulent Flow

The model has been run in the turbulent regime for a Reynolds number of 200000 with an inlet velocity. The results from these runs have been extracted and been presented in the following discussion. Figure 9 shows the velocity profile at the end section of the 5m pipe model of the MTL. The velocity profile is flat, as is expected for a turbulent flow regime.

Figure 9: Velocity profile at the end section of the 5m straight pipe model of the MTL

Figure 10 shows the temperature profile at the end of the Main Test Section and the start of the recuperator zone of the straight pipe model assumption of the MTL in a turbulent regime. The diffusion in the transverse direction is less prominent for the turbulent flow when compared to the diffusion in the laminar regime. This phenomenon
is not unexpected, as the higher velocities dominate the diffusion in the lateral direction more than in the transverse direction.

Figure 10: Temperature profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL

Figure 11: Concentration profile at the end of main test section and the start of the recuperator zone of the 5m straight pipe model of the MTL
The concentration profile at the same location for the turbulent flow is shown in figure 11. The inlet concentration is 0.0 ppm for this case too and the wall concentration is applied according to figure 2. For this case too it can be observed that the concentration diffusion into the bulk of the fluid is not as conspicuous as in the case of the laminar flow for the reasons explained above.

The various profiles from the simulations seem to be acceptable from the theoretical point of view. But these results do not meet the requirements necessary for standardizing the chosen CFD package for carrying out further studies and analysis on the loop. The results discussed so far show that the trends are as expected, but the accuracy of these results has yet to be determined, which has been elucidated in the following discussion.

The preciseness of the results has been checked by comparing the simulation results with the analytical solution. The parameter of consideration based on which the simulation results have been benchmarked is the corrosion/precipitation rate of the iron on the wall regions of the MTL.

![Figure 12: Corrosion/Precipitation Rate for a Turbulent Open Straight Pipe Model](image)

Assumption of the Materials Test Loop from Analytical Model
Figure 12 shows the graph depicting the corrosion/precipitation rate obtained from analytical calculations on the DELTA loop for the straight pipe model assumption. The corrosion/precipitation rate is calculated using the below given empirical formula.

\[ q = D \frac{\partial c}{\partial y} \cong D \frac{\Delta c}{\Delta y} \]  

(59)

where \( q \) is the corrosion/precipitation rate, \( D \) is the diffusivity; \( \Delta c/\Delta y \) is the concentration gradient between the wall and the fluid.

Figure 13: Corrosion/Precipitation Rate for a Laminar Open Straight Pipe Model
Assumption of the Materials Test Loop from Simulation Model

Figure 13 shows the same plot for a simulated model in the laminar straight pipe model. It can be observed that the trends look exactly same as the trends for the analytical
model. The values do not coincide due to the fact that the analytical models have been run for the turbulent case, where as the figure 13 shows the corrosion/precipitation rate for the laminar flow regime. The main object of comparison, though, is the point of maximum corrosion and precipitation. It is noticeable that the points of the maximal corrosion and precipitation fall in the same region for both the analytical and simulation results.

Figure 14: Corrosion / Precipitation Rate for a Turbulent Open Straight Pipe Model

Assumption of the Materials Test Loop from Simulation Model

The results from the turbulent model have also been extracted and the graph depicting the corrosion/precipitation plot has been plotted and shown in figure 14. A keen observation of figures 12 and 14 shows that the rates of corrosion for both the analytical
and simulated models look fairly close to each other. The points of maximum corrosion and maximum precipitation also fall in the same region as in the case of analytical model. It can be inferred from these above comparisons that the simulated models for the straight pipe model assumption of the MTL look alike and hence the simulation results are reasonable. The next step for benchmarking is to make sure that the results from these models are grid independent.

![Figure 15: Grid Independency Check for a Laminar Straight Pipe Flow](image)

To check the grid independency, three different grid structures for the same case have been considered and the results have been compared for the flows in both the laminar and turbulent regimes. The different grid structures considered have already been discussed in the second chapter. The main parameter of consideration for the grid independency test is
again the corrosion/precipitation rate. The corrosion/precipitation rate for the entire three different grid structures have been plotted one on the top of the other. The figures shown below show these plots for the laminar and turbulent regimes.

Figure 15 shows the grid independency check plot for the flow in the laminar regime. The three different grid structures have been named ‘coarse’, ‘fine’ and ‘finer’. It can be discerned from the plot that all the three grid structures fall exactly on the top of each other from which it could be concluded that the results are grid independent. The velocity, temperature and concentration plots shown above are also the plots from the ‘coarse’ grid and hence are grid independent and accurate.

Figure 16: Grid Independency Check for a Turbulent Straight Pipe Flow
Figure 16 shows the grid independency check plot for the turbulent flow regime. The ‘coarse’, ‘fine’, and ‘finer’ grids refer to the same grid structure as for the case of a laminar flow. For this case too it can be observed that the percentage error in values between the ‘fine’ and ‘finer’ grids is less than 5%, which helps deduce the verity that the results are grid independent.

From the reasonably good contours of the velocity, temperature and concentration, the close synchronization of the analytical and simulation models and the grid independency of the simulation results, it can be inferred that the code is capable of serving the current purpose of further analysis on the MTL simulation.

The benchmarking process is still not complete as the results discussed above deal with an open straight pipe flow, where as the MTL is a close loop flow. This led the way to the next assumption that the MTL is a toroidal loop model, the details of which have been presented in the following discussion. Before going into further details of the closed toroidal loop model, a detailed overview of the parametric studies carried out on the open straight pipe model have been presented in the following section.

3.1.2. Parametric Study

As specified before, a parametric study has been carried out on the open straight pipe model to further investigate the effect of various parameters on the rate of corrosion. The parameters considered for the analysis are Schmidt number, initial oxygen concentration and the temperature gradient across the loop length for the flow in both the laminar and turbulent regimes. The additional parameter that has been considered for the turbulent flow regime is the Reynolds number. The various studies and the results from the
outcome of them have been presented with corresponding headings in the discussion below.

3.1.2.1. Reynolds Number

The variation of Reynolds number highly affects the flow patterns. The flow patterns in-turn effect the diffusion rates and hence the rate of corrosion. To examine these effects, the flow has been modeled with different Reynolds numbers. The studies are mainly concentrated only in the turbulent regime, as the flow in the MTL is turbulent.

![Parametric Study in Reynolds Number for a Turbulent Straight Pipe Model](image)

Figure 17: Parametric study in Reynolds number for a turbulent open straight pipe model

A $K$-$\varepsilon$ model has been used for all the studies with the different Reynolds numbers chosen as 150000, 175000, 225000 and 250000. The other parameters have been chosen
to be same as the ones for the benchmark study. The results from the parametric study have been presented as a form of graph with the corrosion/precipitation rate plotted over the loop length for all the different values of the Reynolds numbers modeled. For comparison purposes, the corrosion/precipitation rate for the case of the benchmark study, for which the Reynolds number is 200000, has also been plotted. The graph is shown in figure 17 with detailed labeling. It can be deduced from the graph that the variation of the corrosion/precipitation rate is not greatly effected by varying the Reynolds number.

3.1.2.2. Schmidt Number

The next parameter considered for analysis on the MTL is the Schmidt number which is the ratio of kinematic viscosity and diffusivity. For the analysis, the Schmidt number has been varied by keeping constant kinematic viscosity and varying the diffusivity. Obviously, there is direct effect of diffusivity change on the rate of corrosion. The different Schmidt numbers considered for the parametric study are 50, 100, 150 and 200. Again, the other parameters have been kept at their original values.

The studies have been modeled for the flow in both the laminar and turbulent regimes. The element of comparison here is again the rate of change of corrosion/precipitation along the loop length. Figures 18 and 19 show the plots of the corrosion/precipitation rate obtained for different Schmidt numbers for the laminar and turbulent flow regimes respectively. The case of Schmidt number = 10, which is the benchmark study case has also been plotted along with the other graphs for comparison.
Parametric Study for the Schmidt Number for a Laminar Open Straight Pipe Model

Figure 18: Parametric study in Schmidt number for a laminar open straight pipe model

Parametric Study in Schmidt Number for a Turbulent Straight Pipe Flow

Figure 19: Parametric study in Schmidt number for a turbulent open straight pipe model
The graphs show that the corrosion/precipitation rate increases with the increase in the Schmidt number. In other words, the decrease in diffusivity increases the corrosion/precipitation, since the kinematic viscosity is kept constant. It is also apparent that the difference between the rates of corrosion decrease with the increase of the Schmidt number, meaning, the variation in the corrosion rate between \( \text{Sc}=50 \) and \( \text{Sc}=100 \) is more than the variation in the rate of corrosion between \( \text{Sc}=100 \) and \( \text{Sc}=150 \).

Hence the corrosion rate should be kept low to control the rate of corrosion/precipitation.

3.1.2.3. Initial Oxygen Concentration

Initial oxygen concentration is the oxygen injected into the LBE in the MTL to deter the rate of corrosion. The process of reducing the corrosion by inducing an oxygen layer in the flow has already been discussed in the previous chapter. To check the mass transfer behavior of the LBE due to the inclusion of oxygen concentration and the variation in the trend due to the change of the oxygen concentration value, a parametric study has been carried out with three different initial oxygen concentrations. The three initial oxygen concentration values considered for the analysis are \( c = 0 \text{ppm}, 0.001\text{ppm}, 0.1\text{ppm} \). The case of \( c=0\text{ppm} \) corresponds to the case where there is no oxygen layer induced in the flow. This gives a visual idea about the effect of applying an oxygen layer in the LBE flow.

For the analytical and simulation models, the wall concentration is a function of initial oxygen concentration given by the equation 11. The analysis has been run in both the laminar and turbulent regimes, the results of which have been deliberated in the following discussion.
Figure 20: Parametric study in the initial oxygen concentration for a laminar open straight pipe model

Figures 20 and 21 show the variation of corrosion/precipitation rate along the loop length with the variation of the initial oxygen concentration for a laminar and turbulent flow regimes respectively. The different lines refer to the different initial oxygen concentrations. It is very obvious from the graphs that the increase in the concentration of oxygen highly reduces the corrosion/precipitation rate. The variation is highly perceptible in the case where an initial concentration has been applied and in the case where there is no oxygen layer in the flow for both the laminar and turbulent flow regimes. These
results back the fact that the application of oxygen layer in the flow of the LBE in an MTL greatly reduces the corrosion of the wall surfaces.

![Parametric Study in Initial Oxygen Concentration in a Turbulent Straight Pipe Flow](image)

Figure 21: Parametric study in the initial oxygen concentration for a turbulent open straight pipe model

3.1.2.4 Temperature Gradient along the Loop Length

The wall temperature gradient is the range of induced temperature on the wall. For example, for the benchmark study, the wall temperature has been varied from 623K – 823K, in which case the temperature gradient is 200K. From equation 11, it is obvious that the wall concentration is a function of the wall temperature along the loop length. Hence the variation of the wall temperature gradient varies the wall concentration which
in-turn affects the corrosion/precipitation rate. Therefore a parametric study on the temperature gradient has been performed to study the mass transfer behavior of the LBE flow. The temperature gradients considered for the study are 50K, 100K, 150K and 250K. For all the above models, the base temperature has been maintained at 623K and the upper temperature has been varied accordingly.

Figure 22 shows the discrepancy of the rate of corrosion/precipitation due to the variation of the temperature gradient along the loop length for the case of a laminar flow regime. Clearly, the increase in the temperature gradient increases the corrosion/precipitation rate. The effect is very prominent and hence it is recommended that the temperature gradient be kept at a minimum possible range.

![Parametric Study for the Temperature Gradient Along the Loop Length for a Laminar Open Straight Pipe Flow](image)

Figure 22: Parametric study in the temperature gradient across the loop length for a laminar open straight pipe model
The corrosion/precipitation rate variation due to the variation of temperature gradient for a turbulent flow regime has been shown in figure 23. The effects in the turbulent regime are similar to the ones in the laminar regime and hence a lowest possible temperature gradient is recommended.

![Parametric Study in Temperature Gradient Along the Loop Length for a Turbulent Straight Pipe Model](image)

**Figure 23**: Parametric study in the temperature gradient across the loop length for a turbulent open straight pipe model

Since the Materials Test Loop is a closed loop and the simulations discussed above are the open straight pipe models, further analysis has to be carried out to account for the closed loop flow simulation. As discussed before, a closed toroidal loop model is the initial assumption for the MTL, the results of which have been discussed below.
3.2. Toroidal Loop Model

The Materials Test Loop, as can be seen from figure 1, is a very complicated geometry and an exact simulation is not feasible. Also, the experimental data is very meager for benchmarking. The previous studies had their best assumption of the MTL limited to a closed straight loop model, which is the only basis of comparison for the simulation results. Hence, for the comparison purposes and as an initial benchmark process, the geometry of the MTL is assumed to be toroidal loop model. Attempts have been made to simulate the MTL as a closed straight loop model. But due to technical difficulties that have been explained in the previous chapter, the closed straight loop model could not be made feasible. The next closest assumption for the MTL is a closed toroidal loop model, due to the fact that toroid with a large radius of curvature could safely be assumed to be a straight pipe, as the body forces become negligible for a large radius of curvature and low velocities. As indicated before, the geometry is considered as 2D, due to symmetry. One of the main difficulties faced, though, by using the toroidal loop model is, a linearly variant temperature profile could not be imposed on the walls. For this reason, the regions, where there was a linear increment or decrement of temperature and concentration on the walls, step increment and step decrement of these variables had to be imposed. The model has been run in the turbulent regime with the mesh distribution of 10 X 2 X 1000. The two divisions in the theta direction have been used for the ease in applying the boundary conditions.

Figures 24, 25 and 26 shows the velocity, temperature and concentration profiles respectively, for the toroidal loop model assumption of the MTL. The model has been run for a turbulent case with a Reynolds number of 2000000.
Figure 24: Velocity profile due to turbulent flow at the main test section in the closed toroidal loop model

Figure 25: Temperature profile due to the turbulent flow at the main test section in the closed toroidal loop model

The part of the loop shown in the figures corresponds to the Main Test Section of the Materials Test Loop. The profiles shown in these figures look fairly reasonable, but the main object of comparison is the corrosion/precipitation profile. The benchmarking process is mainly based on good agreement of the analytical and simulation models.
Figure 26: Concentration profile due to the turbulent flow at the main test section in the closed toroidal loop model

Figure 27: Corrosion/Precipitation Rate for a Turbulent Closed Straight Loop Model

Assumption of the Materials Test Loop

Figure 27 shows the corrosion/precipitation rate obtained by analytical studies for a closed straight loop model. By comparing figures 12 and 27, it can be perceived that the
trends look exactly similar excepting that there is a slight shift in the values. This is primarily due to the loop condition in the latter case.

Figure 28: Corrosion/Precipitation Rate for a Turbulent Closed Toroidal Loop Model

Assumption of the Materials Test Loop

The extracted result of the corrosion/precipitation for the simulated closed toroidal loop model is shown in figure 28. The effect of the approximation of a step input is clearly visible as the rise of the concentration flux is not uniform. Though the maximal corrosion and precipitation regions seemed to be in good agreement with the analytical results, as can be seen from the figure, the graphs showed a few peaks and valleys in the areas where step increment/decrement was approximated for linear increment/decrement. The peculiar behavior of a sudden rise and fall at the starting and the end of the loop is due to the inclusion of the momentum source term to simulate the pump. The fluctuations
in the corrosion/precipitation rate restrain this model from being benchmarked for further analysis.

3.3. Rectangular Loop Model

As explained in the previous section, the assumption of the MTL as a toroidal loop did not yield good results, due to the step input approximation for wall temperature. The next closest assumption for the MTL is a closed rectangular loop model with a circular cross section. Because of the non-symmetry, and due to the active participation of the secondary flows due to the elbows present in the rectangular loop model, the geometry can no longer be solved as 2D problem. Hence a 3D model has been considered for this case. The region near the wall has been greatly refined for the reasons explained before.

The following discussion presents the details of the benchmark and parametric studies on the rectangular loop model assumption of the MTL.

3.3.1. Benchmark Study

This section sheds light on the velocity, temperature and concentration profiles obtained by assuming the MTL as a rectangular loop model. The results are shown for the flow in both the laminar and turbulent regimes, which is followed by the comparison of the analytical and simulation results. Finally, the results are shown to be grid independent.

3.3.1.1 Laminar Flow

The model has been run with the boundary conditions specified in the second chapter with the inlet velocity of 0.004m/s resulting in a Reynolds number of 2000. Figure 29
shows the velocity profile at a diametrical section cut along the loop length. The velocity along the whole loop length is shown in the figure. The velocity profiles look reasonable, as the parabolic profiles have been seen in the straight run of the loop. There is a slight eccentricity in the center of the parabola, which can be explained as due to the presence of the elbows which causes the disturbance in the flow.

The velocity at the elbow section is shown separately in the figure 30. The elbow section shown in the figure is in the region of the main test section of the LBE. The figure shows the diametrically cut away section at the elbow.

Figure 29: Velocity Profile in the Overall Loop Length for a Laminar Rectangular Loop Model
Figure 30: Velocity Profile at an Elbow Section of the Laminar Rectangular Loop Model

Figure 31: Temperature Profile in the Overall Loop Length for a Laminar Rectangular Loop Model
Figure 32: Concentration Profile in the Overall Loop Length for a Laminar Rectangular Loop Model

Figure 33: Concentration Profile at an elbow section for a Laminar Rectangular Loop Model
A similar argument applies for the wall concentration diffusion, which is shown in the figures 32 and 33 at the same two locations described above. The figures shown are the section views cut along the diameter of the loop. The wall temperature and concentration are imposed according to figure 2.

![Corrosion/Precipitation Rate for a Laminar Rectangular Loop Model](image)

**Figure 34:** Corrosion/Precipitation rate for a laminar closed rectangular loop model

assumption of the Materials Test Loop

It can be inferred from the above figures that the profiles of the various thermal hydraulic profiles and the mass transfer profiles show the trends as expected. The results still need to be compared with the analytical results to strengthen the above statement. The parameter of comparison remains the corrosion/precipitation rate along the loop length and has been shown in figure 27. The plot obtained for the same parameter using
the simulation model is shown in figure 34. A keen observation of the two figures helps deduce the fact that the trends from both the analytical and simulated models look very similar excepting for a few sections, the reasons of which has been elaborated in the following discussion. The maximum and minimum corrosion rate values do not coincide due to the difference in the flow regimes for the analytical and simulation models.

In figure 34, the graph has two different line patterns. The solid line corresponds to the corrosion/precipitation rate along the whole length of the loop, whereas the dotted lines correspond to the elbow sections of the loop. These sections have been highlighted to illustrate the effect of the elbow sections on the corrosion rate. It is a well-known fact that the secondary flows act in an elbow section and this causes the disruption in the diffusivity of the temperature and concentration. It should be mentioned here that the concentration gradient has been calculated by averaging at four different points that are located on the inside, outside and the two sides on the circumference of the circular cross section along the loop length. This gives a more precise value than choosing a single point for calculating the corrosion rate. Comparison of figures 27 and 34 also show that the difference in patterns is primarily at the elbow sections and the sections after the elbow. One other point of variation is at the section slightly downstream from the zero length. A steep dip in the corrosion rate can be seen at this point. This dip is caused due to the momentum source term incorporated to replicate the pump.

For presenting a detailed insight into the effect of velocity variations on the diffusion of the mass transfer from the wall into the bulk flow at the elbow sections, the velocities and concentrations along the four points mentioned above at one elbow section have been
plotted separately. Also extracted are the velocity and concentration contours at three different cut away sections of the elbow normal to the flow.

Figure 35: Velocity contour at the first elbow cut away section normal to the flow

Figure 36: Concentration profile at the first elbow cut away section normal to the flow
Figures 35 and 36 show the velocity and concentration profile at a section sliced normal to the flow in the elbow in the region of main test section. This section is located geometrically at a few cells downstream after the elbow section begins. The top edge in the figure corresponds to the inside edge of the elbow and the bottom edge in the figure corresponds to the outer edge of the elbow section.

Figures 37 through 40 show the velocity and concentration profiles at the section slices along the elbow further downstream. Figures 37 and 38 are geometrically located at the middle of the elbow and the figures 39 and 40 are at the end of the elbow section. As anticipated, the inside edge of the sections of the elbow have higher dissemination rate than the outside edge.

Figure 37: Velocity contour at the second elbow cut away section normal to the flow
Figure 38: Concentration profile at the second elbow cut away section normal to the flow

Figure 39: Velocity contour at the third elbow cut away section normal to the flow
Figure 40: Concentration profile at the third elbow cut away section normal to the flow

The figures 41 and 42 depict the velocities and concentrations plotted at the three edges of an elbow, namely inside edge, outside edge, and the edge on the side along the flow direction. These figures make obvious the fact that the increment of the velocities result in decrease in the rate of corrosion.
Figure 41: Velocity profile on the edges of the elbow section

Figure 42: Rate of corrosion change on the edges of an elbow section
The detailed deliberation of the effect of the secondary flows at the elbow sections and the consequent variation in the diffusivity justifies the peculiar trend of the corrosion/precipitation rate at the elbow sections in figure 34. Hence, it could be concluded that the results of the simulation are fairly accurate. But before any further analysis could be carried out, it should be made sure that the results are grid independent. The following confabulation outlines the grid independency test.

The process of grid independency check is similar to the method adopted for the grid independency test of the open straight pipe model. Three different grid structures outlined in the previous chapter have been used for running the same analysis.

![Grid Independency Check - Laminar Rectangular Loop Model](image)

Figure 43: Grid Independency Check for a Laminar Rectangular Loop Model
Figure 43 shows the result from the grid independency check. The values on the inside edge, outside edge and the edges on the two sides have been averaged for all the three grid structures and overlaid in the same graph. It can be seen from the figures that the results are grid independent. The ‘fine’ and ‘finer’ grid structures stay almost on the top of each other. For this reason, the ‘finer’ grid structure has been incorporated for the results discussed above and for further analysis.

3.3.1.2. Turbulent Flow

The model has been run for a turbulent flow regime with an inlet velocity of 0.4m/s and a Reynolds number of 200000. Figures 44 and 45 show the velocities at a section cut diametrically over the whole loop length and at an elbow section. The elbow section is physically located at the main test section of the MTL.

![Figure 44: Velocity profile in the overall loop length for a turbulent rectangular loop Model](image)
Figure 45: Velocity profile at an elbow section for a turbulent rectangular loop model

Figure 46: Temperature profile in the overall loop length for a turbulent rectangular loop Model
Figure 46 shows the temperature profile at a diametrical section along the loop length. It is noticeable that the temperature diffusion from the wall into the bulk of the fluid is not as significant as it is for the case of a laminar flow. This is essentially due to the more prominent velocities in the former case than the latter case. The higher velocities in the turbulent flow make the diffusion more predominant in the lateral direction than the transverse direction.

![Temperature profile at a diametrical section along the loop length](image)

Figure 47: Temperature profile at an elbow section for a turbulent rectangular loop model

Temperature distribution in an elbow cut away section is shown in the figure 47. For the turbulent case too the wall temperature and concentration profiles are imposed according to figure 2.

The concentration profiles at the above two locations are shown in figures 48 and 49. The reasoning of the lower diffusion rate in the transverse direction than the lateral
direction applies for the case of corrosion too. This results in a uniform mixing of the concentration in the case of a turbulent flow.

Figure 48: Concentration profile in the overall loop length for a turbulent rectangular loop Model

Figure 49: Concentration profile at an elbow section for a turbulent rectangular loop model
As discussed previously, the next step towards benchmarking is the comparison of the analytical results with the simulation results. Figure 50 shows the corrosion/precipitation rate for the turbulent rectangular loop model assumption of the MTL from the simulation. For this case also, the concentration has been averaged at four different edges of the circular cross section, namely, the inner edge, the outer edge and the edges on the two sides. This has to be compared with the figure 27, which shows the analytical result for a turbulent closed straight loop model assumption. Close observation of these two figures reveals that the curve patterns look alike excepting at a few sections. The amount of corrosion/precipitation rate in cm/yr also coincides closely with the analytical results. The discrepancies in the trends are distinguishable mainly at the elbow regions and at the region where the momentum source has been applied. The elbow regions have been highlighted in the figure for a better sagacity.

From the figure 50, it is lucid that there is an increase in the rate of corrosion/precipitation at one elbow region and there is a decrease in the other three regions. The elbow region where there is an increase in the value falls in the corrosion zone and the other regions where there is a decrease in the value falls in the precipitation zone. In other words, both the rate of corrosion and the rate of precipitation increase in their respective zones, which helps deduce the detail that the elbow regions and the secondary flows formed in these regions intensify the effect of corrosion and precipitation in their respective regions.
Figure 50: Corrosion/Precipitation rate for a turbulent closed rectangular loop model assumption of the Materials Test Loop

Figure 51: Velocity profile on the edges of the elbow section
To authenticate the above conclusion a more comprehensive study on one of the elbow regions has been performed. The edges specified above (inner edge, outer edge, edge on the side) have been taken into consideration and the velocity and concentration profiles at these three edges have been plotted. Figure 51 shows the velocity variation in the flow direction in the elbow region at the three different edges pointed out above. At the same locations, the corrosion rates have been plotted in a graph that is shown in figure 52. By comparing these two figures, it can be excogitated that the increase in velocity increases the corrosion rate and the decrease in velocity decreases the corrosion rate. This is true in the case of precipitation rate also, where the increase / decrease in velocity increases / decreases the precipitation rate respectively.

Figure 52: Corrosion/Precipitation rate on the edges of the elbow section
Further insight into the secondary flows in the elbow section has been provided in the following discussion. Three different cut away sections normal to the flow direction have been shown below. The sections are located at the start, middle and end locations of the elbow present at a section analogous to the main test section of the MTL.

![Velocity contour at the first elbow cut away section normal to the flow](image)

Figure 53: Velocity contour at the first elbow cut away section normal to the flow

The streamline velocity contours and concentration profiles at these three locations have been presented in the figures 53 through 58. Figures 53 and 54 show the velocity contour and concentration profile at the starting location of the elbow section. It can be seen that the secondary flows start developing eddies in the region. And the higher concentration zones, as can be seen, correspond to the higher velocity regions, which further invigorate the statement above.
Figure 54: Concentration profile at the first elbow cut away section normal to the flow

Figure 55: Velocity contour at the second elbow cut away section normal to the flow
Figures 55 and 56 show the velocity and concentration of the section of the elbow further downstream. The secondary flows develop further and result in higher concentration on the inside edge of the elbow. This section is located at the middle of the elbow.

Figure 56: Concentration profile at the second elbow cut away section normal to the flow

Figures 57 and 58 show the velocity and concentration at the end of the elbow section. The higher concentration zone advances more towards the center when compared with the previous two sections of the elbow due to eddies.
Figure 57: Velocity contour at the first elbow cut away section normal to the flow

Figure 58: Concentration profile at the first elbow cut away section normal to the flow
The above deliberation theorizes the active participation of the secondary flows in the corrosion of the MTL and the good tune of the simulation results with the analytical results lays good foundation for the benchmarking process. The final check, though, for the benchmarking process is to check for the dependency of the obtained results on the grid structure. Figure 59 shows the graph depicting the grid independency check. Similar procedure of considering three different grid structures and running the model with the same boundary conditions has been followed. The corrosion/precipitation rate from all the three runs has been compared. It can be seen that the results do not vary by a lot with the change in grid structure. The percentage error in the ‘fine’ and ‘finer’ grids seem to be in a better agreement than the ‘coarse’ grid. Hence it could be concluded that the results from the ‘fine’ grid structure are independent of mesh distribution.

Figure 59: Grid independency check for a turbulent rectangular loop model
This study helps deduce the fact that the simulation results are in good tune with the analytical results and hence the process of benchmarking the CFD code is successful. The research has then been extended to further analyze the effect of various parameters on the mass diffusion, which has been outlined in the following section.

3.3.2. Parametric Study

A parametric study has been carried out for the rectangular loop model with Reynolds number, Schmidt number, initial oxygen concentration and temperature variation along the loop length as parameters. The studies have been carried out both in the laminar and turbulent regimes. The parametric studies are mainly useful in determining the most critical points in the MTL i.e. the points of maximal or minimal corrosion and helps decide on the most favorable parameters to run the loop with longest possible life. The parametric study cases for each parameter have been analyzed separately in the following discussion.

3.3.2.1. Reynolds Number

Reynolds number plays a very vital role in the area of thermal hydraulics. It directly influences the mass diffusion rate in a pipe flow. The mass diffusion rate in turn affects the corrosion or precipitation rate in the MTL. Hence, the behavioral study of the mass diffusion with the variation of velocity makes a very interesting topic for the present case. For this reason, a parametric study of the Reynolds number has been carried out. The studies were limited to the turbulent flow because of the fact that the flow effects on mass diffusion are more predominant for high Reynolds numbers than for the low Reynolds numbers.
The parametric study consisted of flow modeling at five different Reynolds numbers. The range of Reynolds numbers considered were: 150000, 175000, 200000, 225000, and 250000. The simulations were carried out with all the remaining parameters kept at the pre-defined values for the benchmark study. Since the main focus of study is the corrosion/precipitation rate, the results of these rates have been extracted. These results, from all the runs have been plotted against the non-dimensional loop length, as shown in the figure 60.

As can be seen, the concentration flux from all the five runs almost overlap excepting at a few places. The maximal corrosion/precipitation point almost stays the same for all the runs. The only region where the variation is considerable is the region after the point
of maximal corrosion and before the point of minimal corrosion. An elbow is present in this region and the region where the elbow is present has the maximum effect on the corrosion/precipitation rate. Apart from that, the effect of the Reynolds number in the given range is negligible on the corrosion/precipitation rate.

3.3.2.2. Schmidt Number

The next parameter considered for analysis is the Schmidt number. Schmidt number is the ratio of kinematic viscosity and diffusivity. For the parametric study, the kinematic viscosity has been kept constant and the diffusivity has been varied. The various Schmidt numbers considered were, 10, 50, 100, 150 and 200. The variation in the Schmidt number is expected to greatly influence the corrosion/precipitation rate since it is inversely proportional to the diffusivity. The study has been carried out for both the laminar and turbulent regimes. The other properties of the fluid for the analysis were kept constant and same as the benchmark study runs.

Figure 61, shows the plot of variation of concentration flux with the non-dimensional loop length for laminar flow and figure 62 shows the same plot for the turbulent flow. It can be observed from both the figures that, higher the Schmidt number is higher is the corrosion rate and lower is the precipitation. The points of maximum corrosion and precipitation, of course, are not affected by the variation. Hence, for longevity of the life of the MTL, the Schmidt number should be kept as low as possible.
Figure 61: Parametric study in Schmidt number for laminar rectangular loop model

Figure 62: Parametric study in Schmidt number for a turbulent rectangular loop model
3.3.2.3. Initial Oxygen Concentration

The concentration of wall, as described before, is a function of initial oxygen concentration and temperature. The empirical formula is given by equation 11. The corrosion/precipitation rate is directly proportional to the wall concentration.

Four different initial oxygen concentrations have been considered for the study. The simulations have been run both in the laminar and turbulent regimes. The initial oxygen concentrations that have been considered are 0, 0.0001, 0.001 and 0.1. Figures 63 & 64 show the variation of concentration flux with the variation of initial oxygen concentration for the laminar and turbulent regimes respectively. It can be clearly visualized that the initial oxygen concentration highly affects the overall corrosion/precipitation rate. Higher the oxygen concentration is, higher is the corrosion/precipitation rate.

Figure 63: Parametric Study in Initial Oxygen Concentration for Laminar Flow
The case where the initial oxygen concentration is zero has been analyzed for comparison purposes. It can be seen that introduction of oxygen greatly reduces the corrosion of the steel surfaces.

3.3.2.4. Temperature Variation across the Loop Length

The final parameter considered for the parametric study is the wall temperature variation along the loop length. The wall concentration is a function of wall temperature, given by equation 11. Hence, by varying the wall temperature along the loop length has a direct affect on the wall concentration, which in turn affects the corrosion or precipitation rate. For the benchmark study, the temperature gradient considered was 200°C i.e. 623K – 823K. Five different temperature differences have been considered for doing the
parametric study. The temperature gradients considered were, 50K, 100K, 150K, 200K and 250K. For all the five cases, the base temperature has been maintained at 623K. The imposed wall temperature trend along the loop length is also similar to the figure 2 for all the cases. The remaining parameters have been kept at the original conditions for the analysis. Simulations have been carried out in both laminar and turbulent regimes. Figures 65 & 66 show the plot of corrosion/precipitation rate vs. the Loop length for various temperature ranges along the loop length for the laminar and turbulent regimes respectively.

Figure 65: Parametric study of the Temperature variation along the Loop Length for a Laminar Regime
It can be deduced from the figures that the corrosion rate increases with the increase in the temperature gradient. The effect of temperature on the corrosion is very high. A 50K increase in the temperature highly increases the corrosion/precipitation rate as is obvious from the figure. Hence the temperature gradient should be kept at minimum possible levels for the long run of the loop.
CHAPTER 4

CONCLUSIONS

This work is primarily an extension of work done by Xiaoyi He, Ning Li and Mark Mineev [5]. Literature review showed that experimental data in this area of research is limited and hence the analytical results form the basis for comparison of the simulated models. This study provides detailed effects of secondary flows which were not covered in the analytical models. The results from these runs used to benchmark are in good tune with the analytical results and thus the package has been benchmarked for further research, which included the parametric studies. Also, the effects of the secondary flows due to the presence of the elbows in the rectangular loop model make valid the peculiar behavior of the corrosion rates at these locations. The results from the grid independency for the models helped substantiate the reliability of the results from the runs.

The CFD code used lacks in certain features that restrained the simulation of closed straight pipe model assumption for the MTL as in the case of analytical models. This led the way to the usage of the rectangular loop model that helped analyze the effects of secondary flows.

By and large, the studies helped gain more insight into the flow dynamics; thermal and mass transfer behavior of the Lead Bismuth Eutectic. This could lead the way in running the loop with the parameters that could help the longevity of the loop life and the scope for the research is vast.
BIBLIOGRAPHY


4. Valentina Tcharnotskaria, Curtt Ammerman, Timothy Darling, Joe King, Ning Li, Don Shaw, Leon Snodgrass, Keith Woloshun, Liquid Lead-Bismuth Materials Test Loop, LAUR-01-5051


7. Ning Li, Valentina Tcharnotskaria, Tim Darling, Curtt Ammerman, Xiaoyi He, Joe King, David Harkleroad, Lead-Bismuth Eutectic (LBE) Materials Test Loop (MTL) Test Plan, 2001, LA-UR-01-4866

8. Valentina Tcharnotskaria, Curtt Ammerman, Keith Woloshun, Results from Initial Operation of the LANL DELTA Loop


15. Modi and Seth


18. STAR-CD Manuals
VITA

Graduate College
University of Nevada, Las Vegas

Kanthi Kiran Dasika

Local Address:
   969, E. Flamingo Road, Apt. #116
   Las Vegas, NV 89119

Degrees:
   Bachelor of Engineering, Mechanical Engineering, 1998
   College of Engineering, Andhra University, India

Thesis Title: Chemical Kinetics and Thermal Hydraulics of Lead Bismuth Flow Loops

Thesis Examination Committee:
   Chairperson, Dr. Samir Moujaes, Ph. D.
   Committee Member, Dr. Yitung Chen, Ph. D.
   Committee Member, Dr. Mohammed B Trabia, Ph.D.
   Graduate Faculty Representative, Dr. Jerald Frederick, Ph. D.